

SOME MATHEMATICAL PROBLEMS IN A NEOCLASSICAL THEORY OF ELECTRIC CHARGES

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Dedicated to Roger Temam on the occasion of his 70th birthday.

ABSTRACT. We study here a number of mathematical problems related to our recently introduced neoclassical theory for electromagnetic phenomena in which charges are represented by complex valued wave functions as in the Schrödinger wave mechanics. In the non-relativistic case the dynamics of elementary charges is governed by a system of nonlinear Schrödinger equations coupled with the electromagnetic fields, and we prove that if the wave functions of charges are well separated and localized their centers converge to trajectories of the classical point charges governed by the Newton's equations with the Lorentz forces. We also found exact solutions in the form of localized accelerating solitons. Our studies of a class of time multiharmonic solutions of the same field equations show that they satisfy Planck-Einstein relation and that the energy levels of the nonlinear eigenvalue problem for the hydrogen atom converge to the well-known energy levels of the linear Schrödinger operator when the free charge size is much larger than the Bohr radius.

1. INTRODUCTION

It is well known that the concept of a point charge interacting with the electromagnetic (EM) field has fundamental problems. Indeed, in the classical electrodynamics the evolution of a point charge q of a mass m in an external electromagnetic (EM) field is governed by Newton's equation

$$\frac{d}{dt}[m\mathbf{v}(t)] = q \left[\mathbf{E}(t, \mathbf{r}(t)) + \frac{1}{c} \mathbf{v}(t) \times \mathbf{B}(t, \mathbf{r}(t)) \right] \quad (1)$$

where \mathbf{r} and $\mathbf{v} = \dot{\mathbf{r}} = \frac{d\mathbf{r}}{dt}$ are respectively the charge's position and velocity, $\mathbf{E}(t, \mathbf{r})$ and $\mathbf{B}(t, \mathbf{r})$ are the electric field and the magnetic induction, and the right-hand side of the equation (1) is the Lorentz force. On other hand, if the charge's time-dependent position and velocity are respectively \mathbf{r} and \mathbf{v} then the corresponding EM field is described by the Maxwell equations

$$\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \quad \nabla \cdot \mathbf{B} = 0, \quad (2)$$

$$\frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\frac{4\pi}{c} q\delta(\mathbf{x} - \mathbf{r}(t)) \mathbf{v}(t), \quad \nabla \cdot \mathbf{E} = 4\pi q\delta(\mathbf{x} - \mathbf{r}(t)), \quad (3)$$

where δ is the Dirac delta-function, $\mathbf{v}(t) = \dot{\mathbf{r}}(t)$, c is speed of light. If one would like to consider equations (1)-(3) as a closed system "charge-EM field" there is a problem. Its origin is a singularity of the EM field exactly at the position of

1991 *Mathematics Subject Classification.* 35Q61; 35Q55; 35Q60; 35Q70; 35P30.

Key words and phrases. Maxwell equations, nonlinear Schrödinger equation, Newton's law, Lorentz force, hydrogen atom, nonlinear eigenvalue problem.

Supported by AFOSR grant number FA9550-04-1-0359.

the point charge, as, for instance, for the electrostatic field \mathbf{E} with the Coulomb's potential $\frac{q}{|\mathbf{x}-\mathbf{r}|}$ with a singularity at $\mathbf{x} = \mathbf{r}$. If one wants to stay within the classical electromagnetic theory, a possible remedy is the introduction of an extended charge which, though very small, is not a point. There are two most well known models for such an extended charge: the semi-relativistic Abraham rigid charge model (a rigid sphere with spherically symmetric charge distribution), [35, Sections 2.4, 4.1, 10.2, 13], [32, Sections 2.2], and the Lorentz relativistically covariant model which was studied and advanced in [1], [20, Sections 16], [28], [30], [32, Sections 2, 6], [33], [35, Sections 2.5, 4.2, 10.1], [37]. Poincaré suggested in 1905-1906, [31] (see also [20, Sections 16.4-16.6], [32, Sections 2.3, 6.1- 6.3], [29, Section 63], [33], [37, Section 4.2] and references there in), to add to the Lorentz-Abraham model non-electromagnetic cohesive forces which balance the charge internal repulsive electromagnetic forces and remarkably restore also the covariance of the entire model.

Another well known problem of a physical nature with point charges and the classical electrodynamics is related to the Rutherford planetary model for the hydrogen atom. The planetary model of the hydrogen atom is inconsistent with physically observed phenomena such as the stability of atoms and the discreteness of the hydrogen energy levels. That inconsistency lead as we well know to introduction of non-classical models, such as the Bohr model and later on the Schrödinger's model of the hydrogen atom.

To address the above mentioned problems with the classical electrodynamics we introduced recently in [5], [6] *wave-corpuscle mechanics* (WCM) for charges which is conceived as one mechanics for macroscopic and atomic scales. This model is *neoclassical* in the sense that it is based on the classical concept of the electromagnetic field but an elementary charge is not a point but a *wave-corpuscle* described by a complex-valued scalar wave function ψ with the density $|\psi(t, \mathbf{x})|^2$ which is not given a probabilistic interpretation. The dynamics and shape of a wave corpuscle is governed by a nonlinear Klein-Gordon or a nonlinear Schrödinger equation in relativistic and nonrelativistic cases respectively, and a wave-corpuscle is defined as a special type of solutions to these equations. Consequently an elementary charge in the WCM does not have a prescribed geometry which differs it from the classical Abraham and Lorentz models and more recent developments (see [7], [23], [25], [18], [35] and references therein). Another important difference is that Newton's equations are not postulated as in (1) but rather are derived from the field equations in a non-relativistic regime when charges are well separated and localized. Physical aspects of the model are discussed in detail in [5], [6], where the Poincaré type cohesive forces are constructed somewhat differently then we propose here. The primary focus of this paper is on studies of mathematical properties of the field equations of the WCM.

The paper is organized as follows. In the first two subsections of this Introduction we describe the system relativistic and non-relativistic Lagrangians and the corresponding field equations, and in the third one we consider the relevant nonlinearities and their examples. Importantly, the nonlinearity depends on a size parameter $a > 0$ associated with a free solution (ground state). Section 2 is devoted to remote interaction regimes for many charges. We prove there that in the case of the non-relativistic field equations when $a \rightarrow 0$ (macroscopic limit) the centers of the interacting charges defined by the formula

$$\mathbf{r}^\ell(t) = \int_{\mathbb{R}^3} \mathbf{x} \left| \psi^\ell(t, \mathbf{x}) \right|^2 d\mathbf{x}, \ell = 1, \dots, N,$$

converge to the solutions of Newton's equations with the Lorentz forces if ψ^ℓ remain localized. We also provide examples of exact solutions of the field equations in the form of accelerating solitons for which the localization assumption holds. In Section 3 we study systems of bound charges and time multiharmonic solutions to the field equations. We consider there, in particular, a connection, discovered in a different setting in [12], between the Planck-Einstein energy-frequency relation and the logarithmic nonlinearity as well as some dynamical issues related to the logarithmic nonlinearity closely related to results in [14], [16]. We continue then with a study of a system of two charges with the logarithmic nonlinearity as a model for the hydrogen atom. We prove that if $\kappa = a_1/a \rightarrow 0$, where a_1 is the Bohr radius, then the lower energy levels associated with this model converge to the well known energy levels of the linear Schrödinger operator for the hydrogen atom. The proof is based on an approach developed in [9], [10] with certain modifications.

1.1. Relativistic Lagrangian and field equations. Let us consider a system of N charges interacting directly only with the EM field described by its 4-vector potential (φ, \mathbf{A}) . The charges are described by their wave functions ψ^ℓ with the superscript index $\ell = 1, \dots, N$ labeling them. The EM fields are related to the potentials φ, \mathbf{A} by the following standard relations

$$\mathbf{E} = -\nabla\varphi - \frac{1}{c}\partial_t\mathbf{A}, \quad \mathbf{B} = \nabla \times \mathbf{A}. \quad (4)$$

We introduce now the system Lagrangian \mathcal{L} which is though similar to the one introduced in [5], [6] but differs from it. A different Lagrangian is introduced here in order to get the hydrogen atom frequency spectrum with desired precision. Namely, to every ℓ -th charge is assigned an adjunct potential $(\varphi^\ell, \mathbf{A}^\ell)$ describing its additional degrees of freedom and our relativistic Lagrangian is defined by

$$\begin{aligned} \mathcal{L} \left((\varphi, \mathbf{A}), \left\{ \psi^\ell \right\}_{\ell=1}^N, \left\{ (\varphi^\ell, \mathbf{A}^\ell) \right\}_{\ell=1}^N \right) &= \frac{1}{8\pi} \left[\left(\nabla\varphi + \frac{1}{c}\partial_t\mathbf{A} \right)^2 - (\nabla \times \mathbf{A})^2 \right] \\ &+ \sum_{\ell} \frac{\chi^2}{2m^\ell} \left[\frac{1}{c^2} \left| \tilde{\partial}_t^\ell \psi^\ell \right|^2 - \left| \tilde{\nabla} \psi^\ell \right|^2 - \kappa_{0\ell}^2 \left| \psi^\ell \right|^2 - G^\ell \left(\psi^{\ell*} \psi^\ell \right) \right] \\ &- \sum_{\ell} \frac{1}{8\pi} \left[\left(\nabla\varphi^\ell + \frac{1}{c}\partial_t\mathbf{A}^\ell \right)^2 - (\nabla \times \mathbf{A}^\ell)^2 \right], \end{aligned} \quad (5)$$

where (i) the covariant derivatives are defined by

$$\tilde{\partial}_t^\ell = \partial_t + \frac{iq^\ell (\varphi - \varphi^\ell)}{\chi}, \quad \tilde{\nabla}^\ell = \nabla - \frac{iq^\ell (\mathbf{A} - \mathbf{A}^\ell)}{\chi c}, \quad (6)$$

(ii) ψ^* is complex conjugate to ψ ; (iii) $m^\ell > 0$ is the ℓ -th charge mass, q^ℓ is the value of the charge, $\kappa_{0\ell} = \frac{m^\ell c}{\chi}$, and $\chi > 0$ is a constant similar to the Planck constant $\hbar = \frac{\hbar}{2\pi}$; (iv) $G^\ell (\psi^{\ell*} \psi^\ell)$ is a nonlinearity which will be described below.

The Euler-Lagrange field equations for the Lagrangian \mathcal{L} defined in (5) include, first of all, the Maxwell equations for the EM potentials

$$\nabla \cdot \left(\frac{1}{c} \partial_t \mathbf{A} + \nabla \varphi \right) = -4\pi \sum_{\ell} \rho^{\ell}, \quad (7)$$

$$\nabla \times (\nabla \times \mathbf{A}) + \frac{1}{c} \partial_t \left(\frac{1}{c} \partial_t \mathbf{A} + \nabla \varphi \right) = \frac{4\pi}{c} \sum_{\ell} \mathbf{J}^{\ell}, \quad (8)$$

where the charge densities and currents are defined by

$$\rho^{\ell} = -\frac{q^{\ell} |\psi^{\ell}|^2}{m^{\ell} c^2} \left(\chi \operatorname{Im} \frac{\partial_t \psi^{\ell}}{\psi^{\ell}} + q^{\ell} (\varphi - \varphi^{\ell}) \right), \quad (9)$$

$$\mathbf{J}^{\ell} = \frac{q^{\ell} |\psi^{\ell}|^2}{m^{\ell}} \left(\chi \operatorname{Im} \frac{\nabla \psi^{\ell}}{\psi^{\ell}} - \frac{q^{\ell} (\mathbf{A} - \mathbf{A}^{\ell})}{c} \right). \quad (10)$$

The field equations include similar Maxwell equations for the adjunct potentials

$$\nabla \cdot \left(\frac{1}{c} \partial_t \mathbf{A}^{\ell} + \nabla \varphi^{\ell} \right) = -4\pi \rho^{\ell}, \quad (11)$$

$$\nabla \times (\nabla \times \mathbf{A}^{\ell}) + \frac{1}{c} \partial_t \left(\frac{1}{c} \partial_t \mathbf{A}^{\ell} + \nabla \varphi^{\ell} \right) = \frac{4\pi}{c} \mathbf{J}^{\ell}, \quad \ell = 1, \dots, N, \quad (12)$$

and equations for the wave functions ψ^{ℓ} in the form of nonlinear Klein-Gordon equations

$$-\frac{1}{c^2} \tilde{\partial}_t^{\ell} \tilde{\partial}_t^{\ell} \psi^{\ell} + \tilde{\nabla}^{\ell 2} \psi^{\ell} - G^{\ell \ell} (\psi^{\ell*} \psi^{\ell}) \psi^{\ell} - \kappa_0^2 \psi^{\ell} = 0, \quad \ell = 1, \dots, N. \quad (13)$$

Note that equations (13) for ψ^{ℓ} are coupled to the equations for EM potentials via the covariant derivatives.

The Lagrangian and equations are Lorentz and gauge invariant, and one can verify that defined above ρ^{ℓ} and \mathbf{J}^{ℓ} satisfy conservation/continuity equation

$$\frac{1}{c} \partial_t \rho^{\ell} + \nabla \cdot \mathbf{J}^{\ell} = 0.$$

If we choose the Lorentz gauge

$$\frac{1}{c} \partial_t \varphi + \nabla \cdot \mathbf{A} = 0, \quad \frac{1}{c} \partial_t \varphi^{\ell} + \nabla \cdot \mathbf{A}^{\ell} = 0 \quad (14)$$

for all potentials, equations (7)-(12) take the form

$$\nabla \varphi - \frac{1}{c^2} \partial_t^2 \varphi = - \sum_{\ell=1}^N 4\pi \rho^{\ell}, \quad (15)$$

$$\frac{1}{c^2} \partial_t^2 \mathbf{A} - \nabla^2 \mathbf{A} = \frac{4\pi}{c} \sum_{\ell=1}^N \mathbf{J}^{\ell}, \quad (16)$$

$$\nabla^2 \varphi^{\ell} - \frac{1}{c^2} \partial_t^2 \varphi^{\ell} = -4\pi \rho^{\ell}, \quad (17)$$

$$\frac{1}{c^2} \partial_t^2 \mathbf{A}^{\ell} - \nabla^2 \mathbf{A}^{\ell} = \frac{4\pi}{c} \mathbf{J}^{\ell}, \quad \ell = 1, \dots, N, \quad (18)$$

where $\rho^\ell, \mathbf{J}^\ell$ are defined by (9), (10). Based on the above equations we assume that always

$$(\varphi, \mathbf{A}) = \sum_\ell (\varphi^\ell, \mathbf{A}^\ell). \quad (19)$$

Hence, from now on we assume that in the relativistic case the dynamics of EM fields and charges is determined by equations (17), (18), (9), (10), (13) and according to (19) and (6) the covariant derivatives $\tilde{\partial}_t^\ell$ and $\tilde{\nabla}^\ell$ in (13) involve only fields $(\varphi^{\ell'}, \mathbf{A}^{\ell'})$ with $\ell' \neq \ell$,

$$\tilde{\partial}_t^\ell = \partial_t + \frac{iq^\ell}{\chi} \sum_{\ell' \neq \ell} \varphi^{\ell'}, \quad \tilde{\nabla}^\ell = \nabla - \frac{iq^\ell}{\chi c} \sum_{\ell' \neq \ell} \mathbf{A}^{\ell'}, \quad (20)$$

implying that the adjunct potentials completely compensate the EM self-action for every charge and effectively there is no EM self-interaction (in [5], [6] this kind of compensation was gained by using an additional nonlinear self-interaction).

Let us turn now to the nonlinearities G . We introduce the nonlinearities here the same way as in [5], [6] with an intention to have a rest (ground) state for a single charge in the form of a localized wave function (form factor). Notice that for a single charge evidently $N = 1$, $\varphi - \varphi^\ell = 0$, $\mathbf{A} - \mathbf{A}^\ell = 0$ and we look for the rest solution in the form

$$\psi^\ell(t, \mathbf{x}) = e^{-i\omega_0 t} \psi(\mathbf{x}), \quad \omega_0 = \frac{mc^2}{\chi} = c\kappa_0 \quad (21)$$

with $\mathbf{A}^\ell = 0$. Substituting (21) in (13) yields

$$\begin{aligned} -\nabla^2 \varphi &= 4\pi |\psi|^2, \\ -\nabla^2 \psi + G'(\psi^* \psi) \psi &= 0. \end{aligned}$$

Now we choose a strictly positive, monotonically decreasing radial function $\dot{\psi}$ (ground state) as a parameter for the model and determine the nonlinearity G' from the following *charge equilibrium condition*:

$$-\nabla^2 \dot{\psi} + G' \left(|\dot{\psi}|^2 \right) \dot{\psi} = 0. \quad (22)$$

The above equation allows to determine the nonlinearity G' as long as $\dot{\psi}$ is a strictly positive, smooth and monotonically decreasing function of $r = |\mathbf{x}|$. In Section 1.3 we consider the nonlinearity in more details providing also examples.

Note that using the Lorentz invariance of the system one can easily obtain a solution which represents the charge-field moving with a constant velocity \mathbf{v} simply by applying to the rest solution $(\psi^\ell, \varphi, \mathbf{0})$ the Lorentz transformation (see [5], [6]).

1.2. Non-relativistic Lagrangian and field equations. Our non-relativistic model describes the case of charges moving with non-relativistic velocities and it is set as follows. Using the frequency-shifting substitution (21) with more general $\psi = \psi_\omega^\ell(t, \mathbf{x})$ which depends on (t, \mathbf{x}) we observe that the second time derivative in (13) can be written in the form

$$-\frac{1}{c^2} \tilde{\partial}_t^\ell \tilde{\partial}_t^\ell \psi_\omega^\ell = \frac{1}{c^2} \left(\partial_t + \frac{iq^\ell}{\chi} \varphi_{\neq \ell} \right)^2 \psi_\omega^\ell - 2i \frac{m^\ell}{\chi} \left(\partial_t + \frac{iq^\ell}{\chi} \varphi_{\neq \ell} \right) \psi_\omega^\ell + \kappa_0^2 \psi_\omega^\ell,$$

where

$$\varphi_{\neq\ell} = \sum_{\ell'\neq\ell} \varphi^{\ell'}. \quad (23)$$

We neglect the term with the factor $\frac{1}{c^2}$ and substitute $-2i\frac{m^\ell}{\chi} \left(\partial_t + \frac{iq^\ell}{\chi} \varphi_{\neq\ell} \right) \psi_\omega^\ell + \kappa_0^2 \psi_\omega^\ell$ for the term $-\frac{1}{c^2} \tilde{\partial}_t^\ell \tilde{\partial}_t^\ell \psi_\omega^\ell$ in (13). Consequently, we replace the nonlinear Klein-Gordon equation (13) by the following nonlinear Schrödinger equation (where we denote the frequency shifted ψ_ω^ℓ by ψ^ℓ)

$$i\chi \partial_t \psi^\ell + \frac{\chi^2}{2m^\ell} \left(\tilde{\nabla}^\ell \right)^2 \psi^\ell - \frac{\chi^2}{2m^\ell} G^\ell \left(\psi^{\ell*} \psi^\ell \right) \psi^\ell - q^\ell \varphi_{\neq\ell} \psi^\ell = 0, \quad (24)$$

where $\tilde{\nabla}^\ell$ is given by (20). Since the magnetic fields generated by moving charges also have coefficient $\frac{1}{c}$ we neglect them preserving only the external magnetic fields and replace $\tilde{\nabla}^\ell$ by the covariant gradient $\tilde{\nabla}_{\text{ex}}^\ell$ defined by

$$\tilde{\nabla}_{\text{ex}}^\ell = \nabla - \frac{iq^\ell \mathbf{A}_{\text{ex}}}{\chi c}. \quad (25)$$

So our non-relativistic Lagrangian is

$$\begin{aligned} \hat{\mathcal{L}}_0 \left(\varphi, \left\{ \psi^\ell \right\}_{\ell=1}^N, \left\{ \varphi^\ell \right\}_{\ell=1}^N \right) &= \frac{|\nabla \varphi|^2}{8\pi} + \sum_\ell \hat{L}^\ell \left(\psi^\ell, \psi^{\ell*}, \varphi \right), \\ \hat{L}_0^\ell &= \frac{\chi i}{2} \left[\psi^{\ell*} \partial_t \psi^\ell - \psi^\ell \partial_t \psi^{\ell*} \right] - \frac{\chi^2}{2m^\ell} \left\{ \left| \tilde{\nabla}_{\text{ex}}^\ell \psi^\ell \right|^2 + G^\ell \left(\psi^{\ell*} \psi^\ell \right) \right\} - \\ &\quad - q^\ell \left(\varphi + \varphi_{\text{ex}} - \varphi^\ell \right) \psi^\ell \psi^{\ell*} - \frac{|\nabla \varphi^\ell|^2}{8\pi}, \end{aligned} \quad (26)$$

where $\mathbf{A}_{\text{ex}}(t, \mathbf{x})$ and $\varphi_{\text{ex}}(t, \mathbf{x})$ are potentials of external EM fields, $\psi^{\ell*}$ is complex conjugate of ψ^ℓ . The Euler-Lagrange equations for the electrostatic potentials have the form

$$-\frac{1}{4\pi} \nabla^2 \varphi = \sum_{\ell=1}^N q^\ell \psi^\ell \psi^{\ell*}, \quad (27)$$

$$-\frac{1}{4\pi} \nabla^2 \varphi^\ell = q^\ell \psi^\ell \psi^{\ell*}, \quad \ell = 1, \dots, N. \quad (28)$$

Assuming that φ, φ^ℓ vanish at infinity we obtain a reduced version of (19)

$$\varphi = \sum_\ell \varphi^\ell. \quad (29)$$

Similarly to the relativistic case we assume now that *nonrelativistic equations for dynamics of charges* in the external EM field with potentials $\varphi_{\text{ex}}, \mathbf{A}_{\text{ex}}$ take the form

$$i\chi \partial_t \psi^\ell = -\frac{\chi^2}{2m^\ell} \left(\tilde{\nabla}_{\text{ex}}^\ell \right)^2 \psi^\ell + q^\ell \left(\varphi_{\neq\ell} + \varphi_{\text{ex}} \right) \psi^\ell + \frac{\chi^2}{2m^\ell} [G_a^\ell]' \left(\left| \psi^\ell \right|^2 \right) \psi^\ell, \quad (30)$$

where $\varphi_{\neq\ell}$ is given by (23) and φ^ℓ is determined from the equations

$$\nabla^2 \varphi^\ell = -4\pi q^\ell \left| \psi^\ell \right|^2, \quad \ell = 1, \dots, N. \quad (31)$$

The solution of the above equation is given by the formula

$$\varphi^\ell(t, \mathbf{x}) = q^\ell \int_{\mathbb{R}^3} \frac{|\psi^\ell|^2(t, \mathbf{y})}{|\mathbf{y} - \mathbf{x}|} d\mathbf{y}. \quad (32)$$

The nonlinear self-interaction terms G_a^ℓ in (30) are determined through the charge equilibrium equation (22) and index a indicates the dependence on the *size parameter* $a > 0$ which we introduce by the formula

$$G'_a(s) = a^{-2} G'_1(a^3 s). \quad (33)$$

More detailed discussion of the nonlinearity is given in the following section.

1.3. Nonlinearity, its basic properties and examples. As we have already mentioned, the *nonlinear self interaction function* G is determined from the charge equilibrium equation (22) based on the form factor (free ground state) $\dot{\psi}$. Important features of our nonlinearity include: (i) the boundedness or slow subcritical growth of its derivative $G'(s)$ for $s \rightarrow \infty$ with consequent boundedness from below of the energy; (ii) slightly singular behavior about $s = 0$, that is for small wave amplitudes.

In this section we consider the construction of the function G , study its properties and provide examples for which the construction of G is carried out explicitly. Throughout this section we have

$$\psi, \dot{\psi} \geq 0 \text{ and hence } |\psi| = \psi.$$

We introduce explicitly the dependence of the free ground state $\dot{\psi}$ on the size parameter $a > 0$ through the following representation of the function $\dot{\psi}(r)$

$$\dot{\psi}(r) = \dot{\psi}_a(r) = a^{-3/2} \dot{\psi}_1(a^{-1}r), \quad (34)$$

where $\dot{\psi}_1(r)$ is a function of the dimensionless variable $r \geq 0$. The dependence on a is chosen so that L^2 -norm $\|\dot{\psi}_a(r)\|$ does not depend on a , hence the function $\dot{\psi}_a(r)$ satisfies the charge normalization condition (53) for every $a > 0$. Obviously, definition (34) is consistent with (22) and (33). The size parameter a naturally has the dimension of length. A properly defined spatial size of $\dot{\psi}_a$, based, for instance, on the variance, is proportional to a with a coefficient depending on $\dot{\psi}_1$. The charge equilibrium equation (22) can be written in the following form:

$$\nabla^2 \dot{\psi}_a = G'_a \left(\dot{\psi}_a^2 \right) \dot{\psi}_a. \quad (35)$$

The function $\dot{\psi}_a(r)$ is assumed to be a smooth (at least twice continuously differentiable) positive monotonically decreasing function of $r \geq 0$ which is square integrable with weight r^2 , we assume that its derivative $\dot{\psi}'_a(r)$ is negative for $r > 0$ and we assume it to satisfy the charge normalization condition of the form (53); such a function is usually called in literature a ground state.

Let us look first at the case $a = 1$, $\dot{\psi}_a = \dot{\psi}_1$, $\dot{\varphi}_a = \dot{\varphi}_1$, for which the equation (35) yields the following representation for $G'(\dot{\psi}_1)$ from (35)

$$G'_1 \left(\dot{\psi}_1^2(r) \right) = \frac{(\nabla^2 \dot{\psi}_1)(r)}{\dot{\psi}_1(r)}. \quad (36)$$

Since $\dot{\psi}_1^2(r)$ is a *monotonic* function, we can find its inverse $r = r(\psi^2)$, yielding

$$G'_1(s) = \frac{\nabla^2 \dot{\psi}_1(r(s))}{\dot{\psi}_1(r(s))}, \quad 0 = \dot{\psi}_1^2(\infty) \leq s \leq \dot{\psi}_1^2(0). \quad (37)$$

Since $\dot{\psi}_1(r)$ is smooth and $\partial_r \dot{\psi}_1 < 0$, $G'(|\psi|^2)$ is smooth for $0 < |\psi|^2 < \dot{\psi}_1^2(0)$. If we do not need $G'(s)$ to be smooth, we extend $G'(s)$ for $s \geq \dot{\psi}_1^2(0)$ as a constant, namely

$$G'_1(s) = G'_1(\dot{\psi}_1^2(0)) \text{ if } s \geq \dot{\psi}_1^2(0). \quad (38)$$

The first derivative of such an extension at $s = \dot{\psi}_1^2(0)$ has a discontinuity point. If $\dot{\psi}_a(r)$ is a smooth function of class C^n , $n > 2$, we always can define an extension of $G'(s)$ for $s \geq \dot{\psi}_1^2(0)$ as a bounded function of class C^{n-2} for all $r > 0$ and

$$G'_1(s) = G'_1(\dot{\psi}_1^2(0)) - 1 \text{ if } s \geq \dot{\psi}_1^2(0) + 1. \quad (39)$$

Slowly growing (subcritical) functions $G'(s)$ which are not constant for large s also can be used, see examples below.

In the case of arbitrary size parameter $a > 0$ we define $G'_a(s)$ by formula (33), and this definition is consistent with (34) and (37).

Let us take a look at general properties of $G'(s)$ as they follow from defining them relations (37). In the examples below the function $G'(s)$ is not differentiable at $s = 0$, but if $\dot{\psi}(r)$ decays exponentially or with a power law the nonlinearity $g(\psi) = G'(|\psi|^2)\psi$ as it enters the field equation (30) is differentiable for all ψ including zero, hence it satisfies the Lipschitz condition. For a Gaussian $\dot{\psi}_1(r)$ which decays superexponentially $G'(|\psi|^2)$ is unbounded at zero and $g(\psi)$ is not differentiable at zero. Since $\dot{\psi}(|\mathbf{x}|) > 0$, the sign of $G'_1(|\psi|^2)$ coincides with the sign of $\nabla^2 \dot{\psi}_1(|\mathbf{x}|)$. At the origin $\mathbf{x} = \mathbf{0}$ the function $\dot{\psi}_1(|\mathbf{x}|)$ has its maximum and, consequently, $G'_1(s) \leq 0$ for s close to $s = \dot{\psi}_1^2(0)$. The Laplacian applied to the radial function $\dot{\psi}_1$ takes the form $\frac{1}{r} \frac{\partial^2}{\partial r^2} (r \dot{\psi}_1 |\mathbf{x}|)$. Consequently, if $r \dot{\psi}_1(r)$ is convex at $r = |\mathbf{x}|$ we have $\nabla^2 \dot{\psi}_1(|\mathbf{x}|) \geq 0$. Since $r^2 \dot{\psi}_1(r)$ is integrable, we naturally assume that $|\mathbf{x}| \dot{\psi}_1(|\mathbf{x}|) \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$. Then if the second derivative of $r \dot{\psi}_1(r)$ has a constant sign near infinity, it must be non-negative as well as $G'_1(s)$ for $s \ll 1$. In the examples we give below $G'_1(s)$ has exactly one zero on the half-axis.

Example 1. Consider a form factor $\dot{\psi}_1(r)$ decaying as a power law, namely

$$\dot{\psi}_1(r) = \frac{c_{\text{pw}}}{(1 + r^2)^{5/4}}, \quad (40)$$

where c_{pw} is the normalization factor, $c_{\text{pw}} = 3^{1/2}/(4\pi)^{1/2}$. This function evidently is positive and monotonically decreasing. Let us find now $G'(s)$ based on the relations (37). An elementary computation of $\nabla^2 \dot{\psi}_1$ shows that

$$\begin{aligned} G'(s) &= \frac{15s^{2/5}}{4c_{\text{pw}}^{4/5}} - \frac{45s^{4/5}}{4c_{\text{pw}}^{8/5}}, \\ G(s) &= \frac{75s^{7/5}}{28c_{\text{pw}}^{4/5}} - \frac{25s^{9/5}}{4c_{\text{pw}}^{8/5}}, \text{ for } 0 \leq s \leq c_{\text{pw}}^2. \end{aligned} \quad (41)$$

The extension for $s \geq c_{\text{pw}}^2$ can be defined as a constant or the same formula (41) can be used for all $s \geq 0$ since corresponding nonlinearity has a subcritical growth.

If we explicitly introduce size parameter a into the form factor using (34), we define $G'_a(s)$ by (33). Notice that the variance of the form factor $\dot{\psi}_1^2(|\mathbf{x}|)$ decaying as a power law (40) is infinite.

Example 2. Now we consider an exponentially decaying form factor $\dot{\psi}_1$ of the form

$$\dot{\psi}_1(r) = c_e e^{-(r^2+1)^{1/2}}, \quad c_e = \left(4\pi \int_0^\infty r^2 e^{-2(r^2+1)^{1/2}} dr \right)^{-1/2}. \quad (42)$$

Evidently $\dot{\psi}_1(r)$ is positive and monotonically decreasing. The dependence $r(s)$ defined by the relation (42) is as follows:

$$r = [\ln^2(c_e/\sqrt{s}) - 1]^{1/2}, \quad \text{if } \sqrt{s} \leq \dot{\psi}_1(0) = c_e e^{-1}. \quad (43)$$

An elementary computation shows that

$$-\frac{\nabla^2 \dot{\psi}_1}{\dot{\psi}_1} = \frac{2}{(r^2+1)^{1/2}} + \frac{1}{(r^2+1)} + \frac{1}{(r^2+1)^{3/2}} - 1. \quad (44)$$

Combining (43) with (44) we readily obtain the following function for $s \leq c_e^2 e^{-2}$

$$G'_1(s) = \left[1 - \frac{4}{\ln(c_e^2/s)} - \frac{4}{\ln^2(c_e^2/s)} - \frac{8}{\ln^3(c_e^2/s)} \right]. \quad (45)$$

We can extend it for larger s as follows:

$$G'_1(s) = G'_1(c_e^2 e^{-2}) = -3 \quad \text{if } s \geq c_e^2 e^{-2}, \quad (46)$$

or we can use a smooth extension as in (39). The function $G'_1(s)$ is not differentiable at $s = 0$. At the same time the function $g(\psi) = G'_1(\psi(r))\psi$ if we set $g(0) = 0$ is continuous and $g(\psi)$ is continuously differentiable with respect to ψ at zero and $g(\psi)$ satisfies a Lipschitz condition. The variance of the exponential form factor $\dot{\psi}_1(r)$ is obviously finite. To find $G'_a(s)$ for arbitrary a we use its representation (33).

Example 3. Now we define a *Gaussian* form factor by the formula

$$\dot{\psi}(r) = C_g e^{-r^2/2}, \quad C_g = \frac{1}{\pi^{3/4}}. \quad (47)$$

Such a ground state is called *gausson* in [12]. Elementary computation shows that

$$\frac{\nabla^2 \dot{\psi}(r)}{\dot{\psi}(r)} = r^2 - 3 = -\ln\left(\dot{\psi}^2(r)/C_g^2\right) - 3.$$

Hence, we define the nonlinearity by the formula

$$G'(|\psi|^2) = -\ln\left(|\psi|^2/C_g^2\right) - 3, \quad (48)$$

and refer to it as *logarithmic nonlinearity*. The nonlinear potential function has the form

$$G(s) = \int_0^s \left(-\ln(s'/C_g^2) - 3 \right) ds' = -s \ln s + s \left(\ln \frac{1}{\pi^{3/2}} - 2 \right). \quad (49)$$

Dependence on the size parameter $a > 0$ is given by the formula

$$G'_a(|\psi|^2) = -a^{-2} \ln\left(a^3 |\psi|^2/C_g^2\right) - 3a^{-2}. \quad (50)$$

Obviously $g(\psi) = G'_1(|\psi|^2)\psi$ is continuous for all $\psi \in \mathbb{C}$ if at zero we set $g(0) = 0$ and is differentiable for every $\psi \neq 0$ but is not differentiable at $\psi = 0$ and does not satisfy the Lipschitz condition. Notice also that $g(\psi)$ has a subcritical growth as $|\psi| \rightarrow \infty$.

2. CHARGES IN REMOTE INTERACTION REGIMES

The primary focus of this section is to show that if the size parameter $a \rightarrow 0$ then the dynamics of centers of localized solutions is approximated by the Newton equations with the Lorentz forces. This is done in the spirit of the well known in the quantum mechanics Ehrenfest Theorem, [34, Sections 7, 23]. We also provide as an example explicit wave-corpuscle solutions which have such a dynamics.

As a first step we describe basic properties of the classical solutions of (30), (31). The Lagrangian $\hat{\mathcal{L}}$ is gauge invariant and every ℓ -th charge has a 4-current $(\rho^\ell, \mathbf{J}^\ell)$ defined by

$$\rho^\ell = q |\psi^\ell|^2, \quad \mathbf{J}^\ell = \left(\frac{\chi q^\ell}{m^\ell} \operatorname{Im} \frac{\nabla \psi^\ell}{\psi^\ell} - \frac{q^{\ell 2} \mathbf{A}_{\text{ex}}}{m^\ell c} \right) |\psi^\ell|^2, \quad (51)$$

which satisfies the continuity equations $\partial_t \rho^\ell + \nabla \cdot \mathbf{J}^\ell = 0$ or

$$\partial_t |\psi^\ell|^2 + \nabla \cdot \left(\frac{\chi}{m^\ell} \operatorname{Im} \frac{\nabla \psi^\ell}{\psi^\ell} |\psi^\ell|^2 - \frac{q^\ell}{m^\ell c} \mathbf{A}_{\text{ex}} |\psi^\ell|^2 \right) = 0. \quad (52)$$

Note that \mathbf{J}^ℓ defined by (51) agrees with the definition of the current (10) in the Maxwell equations. Equations (52) can be obtained by multiplying (30) by $\psi^{\ell*}$ and taking the imaginary part. Integrating the continuity equation we see that $|\psi^\ell|^2 = \text{const}$ and we impose the following normalization condition:

$$\|\psi^\ell\|^2 = \int_{\mathbb{R}^3} |\psi^\ell|^2 d\mathbf{x} = 1, \quad t \geq 0, \quad \ell = 1, \dots, N. \quad (53)$$

The motivation for this particular normalization is that this normalization allows $|\psi^\ell|^2 = |\psi_a^\ell|^2$ to converge to a delta-function and, in addition, for this normalization the solution to (31) given by the formula (32) converges to the Coulomb's potential with the value q^ℓ of the charge if $|\psi_a^\ell|^2$ converges to a delta function. The momentum density \mathbf{P}^ℓ for the Lagrangian $\hat{\mathcal{L}}_0$ in (26) is defined by the formula

$$\mathbf{P}^\ell = \frac{i\chi}{2} \left(\psi^\ell \tilde{\nabla}^{\ell*} \psi^{\ell*} - \psi^{\ell*} \tilde{\nabla}^\ell \psi^\ell \right).$$

Note that so defined momentum density \mathbf{P}^ℓ is related with the current \mathbf{J}^ℓ in (51) by the formula

$$\mathbf{P}^\ell(t, \mathbf{x}) = \frac{m^\ell}{q^\ell} \mathbf{J}^\ell(t, \mathbf{x}). \quad (54)$$

We introduce the total individual momenta \mathbf{P}^ℓ for ℓ -th charge by

$$\mathbf{P}^\ell = \int_{\mathbb{R}^3} \mathbf{P}^\ell d\mathbf{x}, \quad (55)$$

and obtain the following equations for the total individual momenta

$$\frac{d\mathbf{P}^\ell}{dt} = q^\ell \int_{\mathbb{R}^3} \left[\left(\sum_{\ell' \neq \ell} \mathbf{E}^{\ell'} + \mathbf{E}_{\text{ex}} \right) |\psi^{\ell'}|^2 + \frac{1}{c} \mathbf{v}^\ell \times \mathbf{B}_{\text{ex}} \right] d\mathbf{x}, \quad (56)$$

where

$$\mathbf{v}^\ell(t, \mathbf{x}) = \frac{1}{m^\ell} \mathbf{P}^\ell(t, \mathbf{x}) = \frac{1}{q^\ell} \mathbf{J}^\ell(t, \mathbf{x}). \quad (57)$$

The external EM fields \mathbf{E}_{ex} , \mathbf{B}_{ex} in (56) corresponding to the potentials φ_{ex} , \mathbf{A}_{ex} are determined by standard formulas (4). Derivation of (56) is rather elementary. Indeed, in the simplest case where $\mathbf{A}_{\text{ex}} = 0$ we multiply (30) by $\nabla\psi^{\ell*}$, take the real part and integrate the result over the entire space using integration by parts. To obtain (56) in more involved general case one can similarly multiply (30) by $\tilde{\nabla}^{\ell*}\psi^{\ell*}$ and then integrate the result by parts using some vector algebra manipulation.

2.1. Newtonian mechanics as an approximation. Let us show now that if the size parameter a is small compared to the macroscopic scale of variation of EM fields, the charge evolution can be described approximately by the Newton equations with the Lorentz forces similar to (1). In this subsection we give a heuristic derivation. Conditions under which this kind of derivation is justified are given in the next section.

We introduce the ℓ -th charge position $\mathbf{r}^\ell(t)$ and velocity $\mathbf{v}^\ell(t)$ as the following spatial averages

$$\mathbf{r}^\ell(t) = \mathbf{r}_a^\ell(t) = \int_{\mathbb{R}^3} \mathbf{x} \left| \psi_a^\ell(t, \mathbf{x}) \right|^2 d\mathbf{x}, \quad \mathbf{v}^\ell(t) = \frac{1}{q^\ell} \int_{\mathbb{R}^3} \mathbf{J}^\ell(t, \mathbf{x}) d\mathbf{x}, \quad (58)$$

where the current density \mathbf{J}^ℓ is defined by (51). We show below that a combination of the continuity equation (52) with the momentum evolution equations (56) imply the following remarkable property: the positions $\mathbf{r}^\ell(t)$ satisfy with a high accuracy Newton's equations of motion for the system of N point charges if the size parameter a is small enough.

Multiplying continuity equation (52) by \mathbf{x} and integrating we find the following identities

$$\frac{d\mathbf{r}^\ell(t)}{dt} = \int_{\mathbb{R}^3} \mathbf{x} \partial_t \left| \psi^\ell \right|^2 d\mathbf{x} = -\frac{1}{q^\ell} \int_{\mathbb{R}^3} \mathbf{x} \nabla \cdot \mathbf{J}^\ell d\mathbf{x} = \frac{1}{q^\ell} \int_{\mathbb{R}^3} \mathbf{J}^\ell d\mathbf{x} = \mathbf{v}^\ell(t), \quad (59)$$

showing that the positions and velocities defined by formulas (58) are related exactly as in the point charge mechanics. Then integrating (54) we obtain the following kinematic representation for the total momentum

$$\mathbf{P}^\ell(t) = \frac{m^\ell}{q^\ell} \int_{\mathbb{R}^3} \mathbf{J}^\ell(t, \mathbf{x}) d\mathbf{x} = m^\ell \mathbf{v}^\ell(t), \quad (60)$$

which also is exactly the same as for the point charges mechanics. Relations (59) and (60) yield

$$m^\ell \frac{d^2 \mathbf{r}^\ell(t)}{dt^2} = m^\ell \frac{d}{dt} \mathbf{v}^\ell(t) = \frac{d\mathbf{P}^\ell}{dt}, \quad (61)$$

and we obtain from (56) the following system of equations of motion for N charges:

$$m^\ell \frac{d^2 \mathbf{r}^\ell(t)}{dt^2} = q^\ell \int_{\mathbb{R}^3} \left[\left(\sum_{\ell' \neq \ell} \mathbf{E}^{\ell'} + \mathbf{E}_{\text{ex}} \right) \left| \psi^{\ell'} \right|^2 + \frac{1}{c} \mathbf{v}^\ell \times \mathbf{B}_{\text{ex}} \right] d\mathbf{x}, \quad \ell = 1, \dots, N, \quad (62)$$

where $\mathbf{E}^{\ell'}(t, \mathbf{x}) = -\nabla\varphi^{\ell'}(t, \mathbf{x})$, \mathbf{E}_{ex} and \mathbf{B}_{ex} are defined by (4).

The derivation of the above system is analogous to the well known in quantum mechanics *Ehrenfest Theorem*, [34, Sections 7, 23], [12]. Now we give a formal derivation of Newton's law of motion. Let us suppose that for every ℓ -th charge density $\left| \psi^\ell \right|^2$ and the corresponding current density \mathbf{J}^ℓ are localized in a -vicinity of

the position $\mathbf{r}^\ell(t)$, and that $|\mathbf{r}^\ell(t) - \mathbf{r}^{\ell'}(t)| \geq \gamma > 0$ with γ independent on a on time interval $[0, T]$. Then if $a \rightarrow 0$ we get

$$|\psi^\ell|^2(t, \mathbf{x}) \rightarrow \delta(\mathbf{x} - \mathbf{r}^\ell(t)), \quad \mathbf{v}^\ell(t, x) = \mathbf{J}^\ell/q^\ell \rightarrow v^\ell(t) \delta(\mathbf{x} - \mathbf{r}^\ell(t)), \quad (63)$$

where the coefficients before the Dirac delta-functions are determined by the charge normalization conditions (53) and relations (58). Using potential representations (32) we infer from (63) the convergence of the potentials φ^ℓ to the corresponding Coulomb's potentials, namely

$$\varphi^\ell(t, \mathbf{x}) \rightarrow \varphi_0^\ell(t, \mathbf{x}) = \frac{q^\ell}{|\mathbf{x} - \mathbf{r}^\ell|}, \quad \nabla_{\mathbf{r}} \varphi^\ell(t, \mathbf{x}) \rightarrow \frac{q^\ell(\mathbf{x} - \mathbf{r}^\ell)}{|\mathbf{x} - \mathbf{r}^\ell|^3} \text{ as } a \rightarrow 0. \quad (64)$$

Hence, when passing to the limit as $a \rightarrow 0$ we can recast the equations of motion (62) as the system

$$m^\ell \frac{d^2 \mathbf{r}^\ell}{dt^2} = \mathbf{f}^\ell + \epsilon_0, \quad (65)$$

where

$$\mathbf{f}^\ell = \sum_{\ell' \neq \ell} q^\ell \mathbf{E}_0^{\ell'} + q^\ell \mathbf{E}_{\text{ex}}(\mathbf{r}^\ell) + \frac{1}{c} \mathbf{v}^\ell \times \mathbf{B}_{\text{ex}}(\mathbf{r}^\ell), \quad \ell = 1, \dots, N,$$

and $\epsilon_0 \rightarrow 0$ as $a \rightarrow 0$. Notice that the terms \mathbf{f}^ℓ in equations (65) coincide with the Lorentz forces and we see that the limit equations of motion obtained from (65) coincide with *Newton's equations of motion* for point charges interacting via the Coulomb forces and with the external EM field via corresponding Lorentz forces, namely

$$m^\ell \frac{d^2 \mathbf{r}^\ell}{dt^2} = - \sum_{\ell' \neq \ell} \frac{q^\ell q^{\ell'} (\mathbf{r}^{\ell'} - \mathbf{r}^\ell)}{|\mathbf{r}^{\ell'} - \mathbf{r}^\ell|^3} + q^\ell \mathbf{E}_{\text{ex}}(\mathbf{r}^\ell) + \frac{1}{c} \mathbf{v}^\ell \times \mathbf{B}_{\text{ex}}(\mathbf{r}^\ell), \quad \ell = 1, \dots, N. \quad (66)$$

The above formal derivation of Newton's equations of motion is very simple, but if implemented with full rigor would require to impose rather high regularity conditions on the solution and rather strong requirements on the convergence to the delta function. Note that we use essentially the fact that the nonlinearity G'_a , that singularly depends on a as $a \rightarrow 0$ according to (33), does not enter the system (62). In the following subsection we rewrite the system (62) in an integral form which allows to pass to the limit under less restrictive assumptions, and also study an important case of a single charge in an external field.

2.2. Single charge in an external EM field. In this section we describe assumptions under which the above derivation of Newton's law with the Lorentz forces for localized charges can be rigorously justified. In the case of many well separated charges every single charge senses all other charges through the sum of their EM field, and it is this feature of the EM interaction makes a problem of a single charge in external EM field of special importance.

We consider a single charge described by (30) with $N = 1$ in an external EM field where $\varphi_{\text{ex}}(t, x)$, $\mathbf{A}_{\text{ex}}(t, x)$ are two times continuously differentiable functions. Now index ℓ takes only one value, but we still keep it to be consistent with our previous notation. We assume that the first spatial derivatives of \mathbf{E}_{ex} and \mathbf{B}_{ex} are bounded uniformly in (t, x) . We also assume that equation (62) holds in a weaker sense which we describe below.

First let us recast (62) in a different form. Multiplying (52) by $\mathbf{x} - \mathbf{r}^\ell(t)$ we obtain

$$\begin{aligned} & m^\ell \partial_t \left(\left| \psi^\ell \right|^2 (\mathbf{x} - \mathbf{r}^\ell(t)) \right) + m^\ell \left| \psi^\ell \right|^2 \partial_t \mathbf{r}^\ell(t) + \\ & + \nabla \cdot \left(\left(\chi \operatorname{Im} \frac{\nabla \psi^\ell}{\psi^\ell} \left| \psi^\ell \right|^2 - \frac{q^\ell}{c} \mathbf{A}_{\text{ex}} \left| \psi^\ell \right|^2 \right) (\mathbf{x} - \mathbf{r}^\ell(t)) \right) \\ & = \chi \operatorname{Im} \frac{\nabla \psi^\ell}{\psi^\ell} \left| \psi^\ell \right|^2 - \frac{q^\ell}{c} \mathbf{A}_{\text{ex}} \left| \psi^\ell \right|^2. \end{aligned}$$

Note that the right-hand side of the above equation coincides with $m^\ell \mathbf{v}^\ell(t, \mathbf{x})$. Substituting this expression for \mathbf{v}^ℓ into (62) (for a single particle) and we get

$$m^\ell \frac{d^2 \mathbf{r}^\ell(t)}{dt^2} = q^\ell \int_{\mathbb{R}^3} \mathbf{E}_{\text{ex}} \left| \psi^\ell \right|^2 d\mathbf{x} + \frac{q^\ell}{c} \partial_t \mathbf{r}^\ell(t) \times \int_{\mathbb{R}^3} \left| \psi^\ell \right|^2 \mathbf{B}_{\text{ex}} d\mathbf{x} + \epsilon_3, \quad (67)$$

where

$$\begin{aligned} \epsilon_3 &= \frac{q^\ell}{c} \int_{\mathbb{R}^3} \partial_t \left(\left| \psi^\ell \right|^2 (\mathbf{x} - \mathbf{r}^\ell(t)) \right) \times \mathbf{B}_{\text{ex}} d\mathbf{x} \\ &+ \frac{q^\ell}{m^\ell c} \int_{\mathbb{R}^3} \nabla \cdot \left[\left(\chi \operatorname{Im} \frac{\nabla \psi^\ell}{\psi^\ell} \left| \psi^\ell \right|^2 - \frac{q^\ell}{c} \mathbf{A}_{\text{ex}} \left| \psi^\ell \right|^2 \right) (\mathbf{x} - \mathbf{r}^\ell(t)) \right] \times \mathbf{B}_{\text{ex}} d\mathbf{x}. \end{aligned} \quad (68)$$

Observe then that according to the charge normalization

$$\begin{aligned} q^\ell \int_{\mathbb{R}^3} \mathbf{E}_{\text{ex}} \left| \psi^\ell \right|^2 d\mathbf{x} &= q^\ell \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t)) + \epsilon_1, \text{ where} \\ \epsilon_1 &= q^\ell \int_{\mathbb{R}^3} (\mathbf{E}_{\text{ex}}(t, \mathbf{x}) - \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t))) \left| \psi^\ell \right|^2 d\mathbf{x}, \end{aligned} \quad (69)$$

and

$$\begin{aligned} \int_{\mathbb{R}^3} \left| \psi^\ell \right|^2 \mathbf{B}_{\text{ex}} d\mathbf{x} &= \mathbf{B}_{\text{ex}}(t, \mathbf{r}^\ell(t)) + \epsilon_2, \text{ where} \\ \epsilon_2 &= \int_{\mathbb{R}^3} (\mathbf{B}_{\text{ex}}(t, \mathbf{x}) - \mathbf{B}_{\text{ex}}(t, \mathbf{r}^\ell(t))) \left| \psi^\ell \right|^2 d\mathbf{x}. \end{aligned} \quad (70)$$

Hence (67) can be written in the form

$$m^\ell \frac{d^2 \mathbf{r}^\ell(t)}{dt^2} = q^\ell \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t)) + \epsilon_1 + \frac{q^\ell}{c} \partial_t \mathbf{r}^\ell(t) \times [\mathbf{B}_{\text{ex}}(t, \mathbf{r}^\ell(t)) + \epsilon_2] + \epsilon_3. \quad (71)$$

2.2.1. *Dynamics in an external electric field.* Here we consider in detail a simpler case where external magnetic field is absent, $\mathbf{A}_{\text{ex}} = 0$. In this case

$$\mathbf{B}_{\text{ex}} = 0, \quad \mathbf{E}_{\text{ex}} = -\nabla \varphi_{\text{ex}}, \quad \epsilon_2 = 0, \quad \epsilon_3 = 0,$$

and the field equations take the form

$$i\chi \partial_t \psi^\ell = -\frac{\chi^2 \nabla^2 \psi^\ell}{2m^\ell} + q\varphi_{\text{ex}} \psi^\ell + \frac{\chi^2}{2m} G'_a \left(\left| \psi^\ell \right|^2 \right) \psi^\ell, \quad (72)$$

$$\nabla^2 \varphi^\ell = -4\pi q \left| \psi^\ell \right|^2. \quad (73)$$

As we already mentioned, in this section index ℓ takes only one value. First, let us recall some properties of equations (72), (73). Note that equation (72) does not involve the potential φ^ℓ and can be solved independently from equation (73). If

the nonlinearity $g(\psi) = G'_a(|\psi|^2)\psi$ is a continuously differentiable function of ψ with uniformly bounded derivative, and φ_{ex} is a smooth bounded function, then the local existence and uniqueness of a solution of (72) with a prescribed initial data in $H^1(\mathbb{R}^3)$ which belongs to and is bounded in $H^1(\mathbb{R}^3)$ is well known, see [15, Remark 4.4.8]. This solution is defined for all $t > 0$ if (110) holds for G^ℓ since the energy

$$\mathbf{E}_0(\psi^\ell) = \int \frac{\chi^2}{2m^\ell} \left\{ |\nabla \psi^\ell|^2 + G^\ell(|\psi^\ell|^2) \right\} + q^\ell \varphi_{\text{ex}} |\psi^\ell|^2 \, dx \quad (74)$$

is bounded from below on the invariant set $\{\psi \in H^1, \|\psi\| = 1\}$. The existence and uniqueness of solutions of the initial value problem for (72) with $\varphi_{\text{ex}} = 0$ and the logarithmic nonlinearity as in (48) were proven in [16], see also [15].

Now we will show that, under a localization assumption, the centers $\mathbf{r}^\ell(t)$ of wave function ψ^ℓ defined by (58) converge to trajectories governed Newton's law of motion for point charges. To eliminate the time derivatives in equation (67) we integrate it twice in time obtaining

$$\mathbf{r}^\ell(t) = \mathbf{r}_0^\ell + \dot{\mathbf{r}}_0^\ell t + \int_0^t \int_0^{t_2} \frac{q^\ell}{m^\ell} \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t_1)) \, dt_1 dt_2 + \epsilon_4, \quad (75)$$

where

$$\begin{aligned} \epsilon_4 &= \frac{1}{m^\ell} \int_0^t \int_0^{t_2} \epsilon_1 \, dt_1 dt_2 \\ &= \frac{1}{m^\ell} \int_0^t \int_0^{t_2} q^\ell \int_{\mathbb{R}^3} (\mathbf{E}_{\text{ex}}(t, \mathbf{x}) - \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t))) |\psi^\ell|^2 \, d\mathbf{x} dt_1 dt_2. \end{aligned} \quad (76)$$

Let us denote $\mathbf{z}(t) = \mathbf{r}^\ell(t) - \mathbf{r}_0^\ell - \dot{\mathbf{r}}_0^\ell t$ and rewrite (75) in the form

$$\mathbf{z} = F(\mathbf{z}) + \epsilon_4, \quad (77)$$

$$F(\mathbf{z}) = \int_0^t \int_0^{t_2} \frac{q^\ell}{m^\ell} \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(0) + \dot{\mathbf{r}}^\ell(0)t + \mathbf{z}) \, dt_1 dt_2.$$

We consider now equation (75) on a small time interval $[0, T]$ with solutions in the space of continuous functions $C([0, T])$. Since the first order spatial derivatives of \mathbf{E}_{ex} are bounded uniformly, the operator F satisfies a global Lipschitz estimate

$$\|F(\mathbf{z}_1) - F(\mathbf{z}_2)\|_{C([0, T])} \leq CT^2 \|\mathbf{z}_1 - \mathbf{z}_2\|_{C([0, T])}. \quad (78)$$

In addition to that we have

$$\|F(\mathbf{z})\|_{C([0, T])} \leq C_1 T^2 \text{ if } \|\mathbf{z}\|_{C([0, T])} \leq 2 |\mathbf{r}^\ell(0)|.$$

Let us take $T > 0$ so small that

$$CT^2 \leq 1/4, \quad C_1 T^2 \leq 1/4, \quad |\dot{\mathbf{r}}^\ell(0)T| \leq |\mathbf{r}^\ell(0)|, \quad (79)$$

and let \mathbf{z}_0 be a solution of the equation $\mathbf{z}_0 = F(\mathbf{z}_0)$ satisfying $\|\mathbf{z}_0\|_{C([0, T])} \leq 2 |\mathbf{r}^\ell(0)|$. Such a solution exists and is unique by the contraction principle. Note then that the corresponding $\mathbf{r}(t) = \mathbf{z}_0(t) + \mathbf{r}_0^\ell + \dot{\mathbf{r}}_0^\ell t$ is a solution of (75) with $\epsilon_4 = 0$ and consequently is a solution of the equation

$$m^\ell \frac{d^2 \mathbf{r}(t)}{dt^2} = q^\ell \mathbf{E}_{\text{ex}}(\mathbf{r}), \quad \mathbf{r}(0) = \mathbf{r}_0^\ell, \quad \frac{d\mathbf{r}(0)}{dt} = \dot{\mathbf{r}}_0^\ell, \quad (80)$$

which coincides with Newton's equation (66) for a single point charge in an external electric field. To estimate a difference between the Newtonian trajectory $\mathbf{r}(t)$ and

the charge position $\mathbf{r}^\ell(t)$ defined by (58) we subtract from (77) equation for \mathbf{z}_0 and obtain

$$\mathbf{z} - \mathbf{z}_0 = F(\mathbf{z}) - F(\mathbf{z}_0) + \epsilon_4.$$

Using (78) and smallness of T we obtain the following inequality

$$\|\mathbf{r}^\ell - \mathbf{r}\|_{C([0,T])} = \|\mathbf{z} - \mathbf{z}_0\|_{C([0,T])} \leq 2\|\epsilon_4\|_{C([0,T])}. \quad (81)$$

The above argument proves the following theorem.

Theorem 2.1. *Suppose that $\mathbf{A}_{\text{ex}}(t, x) = 0$ and $\varphi_{\text{ex}}(t, x)$ are two times continuously differentiable functions, and that the first spatial derivatives of \mathbf{E}_{ex} are bounded uniformly in (t, x) . Suppose also that: (i) there is a family of solutions $\psi^\ell = \psi_a$ of the NLS (72) with $G = G_a$ which depend on the size parameter $a > 0$; (ii) $\mathbf{r}^\ell(t)$ as defined by (58) is a continuous function of $t \in [0, T]$, where T is a sufficiently small fixed number which satisfies (79); (iii) (75) holds where ϵ_4 satisfies the following relation*

$$\begin{aligned} \lim_{a \rightarrow 0} \|\epsilon_4\|_{C([0,T])} &= 0, \text{ where } \|\epsilon_4\|_{C([0,T])} = \\ &= \sup_{t \in [0,T]} \left| \int_0^t \int_0^{t_2} \frac{q^\ell}{m^\ell} \int_{\mathbb{R}^3} (\mathbf{E}_{\text{ex}}(t, \mathbf{x}) - \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t))) |\psi^\ell|^2 d\mathbf{x} dt_1 dt_2 \right|. \end{aligned} \quad (82)$$

Then if $\mathbf{r}(t)$ is a solution of Newton's equation (80) we have

$$\sup_{t \in [0,T]} |\mathbf{r}^\ell(t) - \mathbf{r}(t)| \rightarrow 0 \text{ as } a \rightarrow 0.$$

Note that the function $(\mathbf{E}_{\text{ex}}(t, \mathbf{x}) - \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t))) = 0$ at $\mathbf{x} = \mathbf{r}^\ell$ and it is a bounded differentiable function, implying that condition (82) is a weaker version of convergence $|\psi^\ell|^2(t, \mathbf{x}) \rightarrow \delta(\mathbf{x} - \mathbf{r}^\ell(t))$ in $C(\mathbb{R}^3)^*$ uniformly on $[0, T]$. Since $|\psi^\ell|^2$ for every a satisfy normalization condition (53), the convergence to $\delta(\mathbf{x} - \mathbf{r}^\ell(t))$ means a weak form of localization around $\mathbf{r}^\ell(t)$. In Theorem 2.3 and Remark 3 we give an example where condition (82) holds.

2.2.2. Dynamics in a general external electromagnetic field. Now let us consider the case when the external magnetic field described by its vector potential \mathbf{A}_{ex} does not vanish. For localized solutions of equation (30) where $N = 1$ and ℓ takes one value we want to derive the convergence of $\mathbf{r}^\ell(t)$ defined by (58) to a solution of Newton's equation of motion

$$m \frac{d^2 \mathbf{r}}{dt^2} = q \mathbf{E}_{\text{ex}}(t, \mathbf{r}) + \frac{q}{c} \frac{d\mathbf{r}}{dt} \times \mathbf{B}_{\text{ex}}(t, \mathbf{r}). \quad (83)$$

Considering equation (71) as a perturbation of equation (83) let us estimate the difference between their solutions. First we derive from equation (71) estimates for $(\partial_t \mathbf{r}^\ell(t))^2$ similar to usual energy estimates. Multiplying (71) by $\partial_t \mathbf{r}^\ell(t)$ we obtain

$$m^\ell \partial_t^2 \mathbf{r}^\ell(t) \partial_t \mathbf{r}^\ell(t) = q^\ell \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t)) \partial_t \mathbf{r}^\ell(t) + (\epsilon_1 + \epsilon_3) \partial_t \mathbf{r}^\ell(t).$$

Integration of the above equation with the respect to t yields

$$\begin{aligned} \frac{m^\ell}{2} \left[(\partial_t \mathbf{r}^\ell(t))^2 - (\partial_t \mathbf{r}^\ell(0))^2 \right] &= \\ &= \int_0^t q^\ell \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t_1)) \partial_t \mathbf{r}^\ell(t_1) + (\epsilon_1 + \epsilon_3) \partial_t \mathbf{r}^\ell(t_1) dt_1. \end{aligned} \quad (84)$$

Hence

$$\begin{aligned} (\partial_t \mathbf{r}^\ell(t))^2 &\leq (\partial_t \mathbf{r}^\ell(0))^2 + 2M \left[\int_0^t (\partial_t \mathbf{r}^\ell(t_1))^2 dt_1 \right]^{1/2} \\ &\leq (\partial_t \mathbf{r}^\ell(0))^2 + M^2 + \int_0^t (\partial_t \mathbf{r}^\ell(t_1))^2 dt_1, \end{aligned}$$

where

$$M^2 = \int_0^t \left(\frac{q^\ell}{m^\ell} \mathbf{E}_{\text{ex}}(t, \mathbf{r}^\ell(t_1)) + \frac{(\epsilon_1 + \epsilon_3)}{m^\ell} \right)^2 dt_1. \quad (85)$$

Consequently,

$$(\partial_t \mathbf{r}^\ell(t))^2 \leq M_1 \text{ for } t \in [0, T], \quad (86)$$

where constant M_1 depends on constants M and T . Let $\mathbf{r}(t)$ be a solution of (83) with initial data

$$\mathbf{r}(0) = \mathbf{r}^\ell(0), \quad \frac{d\mathbf{r}}{dt}(0) = \frac{d\mathbf{r}^\ell}{dt}(0). \quad (87)$$

In a similar way we obtain inequality (86) for $(\partial_t \mathbf{r}(t))^2$ with a constant $M_1 = M_{10}$ which does not depend on $\epsilon_1 + \epsilon_3$. To estimate the difference $\mathbf{r}^\ell - \mathbf{r}$ we subtract (83) from (71), multiply the difference by $\partial_t(\mathbf{r}^\ell - \mathbf{r})$ and integrate the result with respect to t obtaining

$$\begin{aligned} \frac{m^\ell}{2} (\partial_t(\mathbf{r}^\ell - \mathbf{r}))^2 &= \int_0^t q^\ell (\mathbf{E}_{\text{ex}}(t_1, \mathbf{r}^\ell) - \mathbf{E}_{\text{ex}}(t, \mathbf{r})) \partial_t(\mathbf{r}^\ell - \mathbf{r}) dt_1 \\ &\quad + \frac{q^\ell}{c} \int_0^t \partial_t \mathbf{r} \times (\mathbf{B}_{\text{ex}}(t, \mathbf{r}^\ell(t)) - \mathbf{B}_{\text{ex}}(t, \mathbf{r}(t))) \partial_t(\mathbf{r}^\ell - \mathbf{r}) dt_1 \\ &\quad + \int_0^t \left(\frac{q^\ell}{c} \partial_t \mathbf{r}^\ell(t) \times \epsilon_2 + \epsilon_1 + \epsilon_3 \right) \partial_t(\mathbf{r}^\ell - \mathbf{r}) dt_1. \end{aligned} \quad (88)$$

Therefore, using inequality (86) for $(\partial_t \mathbf{r}(t))^2$ and $(\partial_t \mathbf{r}^\ell(t))^2$, we obtain

$$\begin{aligned} (\partial_t(\mathbf{r}^\ell - \mathbf{r}))^2 &\leq \left(2C \frac{q^\ell}{m^\ell} + \frac{q^\ell}{m^\ell c} 2CM_{10} \right) \int_0^t |\mathbf{r}^\ell - \mathbf{r}| |\partial_t(\mathbf{r}^\ell - \mathbf{r})| dt_1 \\ &\quad + 2 \int_0^t \left(\frac{q^\ell}{m^\ell c} M_1 |\epsilon_2| + |\epsilon_1 + \epsilon_3| \right) |\partial_t(\mathbf{r}^\ell - \mathbf{r})| dt_1. \end{aligned} \quad (89)$$

Using an elementary inequality

$$|\mathbf{r}^\ell - \mathbf{r}| = \left| \int_0^t \partial_t(\mathbf{r}^\ell - \mathbf{r}) dt_1 \right| \leq t^{1/2} Z^{1/2}(t), \quad (90)$$

where

$$Z(t) = \left(\int_0^t (\partial_t(\mathbf{r}^\ell - \mathbf{r}))^2 dt_1 \right), \quad (91)$$

we obtain from (89) for $t \in [0, T]$

$$\begin{aligned} (\partial_t(\mathbf{r}^\ell - \mathbf{r}))^2 &\leq \left(2C \frac{q^\ell}{m^\ell} + \frac{q^\ell}{m^\ell c} 2CM_{10} \right) \int_0^t t_1^{1/2} Z^{1/2}(t_1) |\partial_t(\mathbf{r}^\ell - \mathbf{r})| dt_1 \\ &\quad + 2 \left[\int_0^t (\partial_t(\mathbf{r}^\ell - \mathbf{r}))^2 dt_1 \right]^{1/2} \left[\int_0^t \left(\frac{q^\ell}{m^\ell c} M_1 |\epsilon_2| + |\epsilon_1 + \epsilon_3| \right) dt_1 \right]^{1/2} \\ &\leq 2^{1/2} C t \frac{q^\ell}{m^\ell} Z(t) + 2 Z^{1/2}(t) \epsilon_5, \end{aligned} \quad (92)$$

where

$$\epsilon_5 = \left[\int_0^T \left(\frac{q^\ell}{m^\ell c} M_1 |\epsilon_2| + |\epsilon_1 + \epsilon_3| \right)^2 dt_1 \right]^{1/2}.$$

Rewriting inequality (92) in the form

$$\partial_t Z \leq 2^{1/2} C t \frac{q^\ell}{m^\ell} Z + 2 Z^{1/2} \epsilon_5,$$

we obtain the following inequality

$$Z^{1/2} \leq \frac{\epsilon_5}{C_2} (e^{C_2 t} - 1) \text{ for } t \in [0, T],$$

with a constant C_2 which does not depend on ϵ_5 . Hence $Z(t) \rightarrow 0$ as $\epsilon_5 \rightarrow 0$, and using inequalities (90) and (92) we conclude that $|\mathbf{r}^\ell - \mathbf{r}| \rightarrow 0$ and $(\partial_t (\mathbf{r}^\ell - \mathbf{r}))^2 \rightarrow 0$ as $\epsilon_5 \rightarrow 0$.

The above argument proves the following theorem.

Theorem 2.2. *Suppose that $\mathbf{A}_{\text{ex}}(t, \mathbf{x})$ and $\varphi_{\text{ex}}(t, \mathbf{x})$ are two times continuously differentiable functions, and that the first spatial and time derivatives of \mathbf{E}_{ex} and \mathbf{B}_{ex} are bounded uniformly in (t, \mathbf{x}) for $t \in [0, T], \mathbf{x} \in \mathbb{R}^3$. Suppose also that (i) there is a family of solutions $\psi^\ell = \psi_a$ of the NLS equations (30) with $N = 1$, $G = G_a$ which depend on the size parameter $a > 0$; (ii) $\mathbf{r}^\ell(t)$ and $\partial_t \mathbf{r}^\ell(t)$ as defined by (58) are continuous functions of $t \in [0, T]$; (iii) equality (88) holds, and M defined by (85) is bounded uniformly in a , $0 < a \leq a_0$; (iv) the following limit relation holds*

$$\int_0^T \left(\frac{q^\ell}{m^\ell c} M_1 |\epsilon_2| + |\epsilon_1 + \epsilon_3| \right)^2 dt_1 \rightarrow 0 \text{ as } a \rightarrow 0, \quad (93)$$

where $\epsilon_1, \epsilon_2, \epsilon_3$ are defined by (69), (70), (68), M_1 is a constant which depends on M .

Then if $\mathbf{r}(t)$ satisfies Newton's equation (83) we have

$$\sup_{t \in [0, T]} |\mathbf{r}^\ell(t) - \mathbf{r}(t)| \rightarrow 0, \quad \sup_{t \in [0, T]} |\partial_t \mathbf{r}^\ell(t) - \partial_t \mathbf{r}(t)| \rightarrow 0 \text{ as } a \rightarrow 0.$$

Remark 1. Note that the derivation of Newton's law of motion for charge centers in Theorems 2.1 and 2.2 does not depend explicitly on the particular nonlinearity G and the value of $\chi > 0$. Analysis of the hydrogen atom model in Section 5.1 shows that $\chi = \hbar$ is a natural choice.

Remark 2. Theorems similar to Theorems 2.1 and 2.2 for a system of interacting charges can be analogously formulated and proven. Among additional conditions one has to assume the condition of non-collision, that is the trajectories of Newton's system (66) have to be separated on the time interval $[0, T]$: $|\mathbf{r}^\ell(t) - \mathbf{r}^{\ell'}(t)| \geq d > 0$ if $\ell \neq \ell'$ with a constant d which does not depend on a . Note that one cannot assume that the electrostatic potentials $\varphi^{\ell'}$ have uniformly bounded gradients uniformly in a since they converge to the Coulomb potentials. But looking at (82) where \mathbf{E}_{ex} is replaced by $-\nabla \varphi_{\text{ex}} - \nabla \varphi_{\neq \ell}$ we observe that uniform boundedness of $\nabla \varphi^{\ell'}$ is required only in a vicinity of $\mathbf{r}^\ell(t)$ with a fixed radius $d/2$, whereas outside the vicinity a natural assumption is convergence to zero of the integral of $|\psi^{\ell'}|^2 |\nabla \varphi_{\neq \ell}|$.

2.2.3. *Exact wave-corpuscle solutions: accelerating solitons.* Here we consider the field equations (30), (31) for a single charge, omitting the index ℓ , and present a family of their exact solutions in the form of accelerating solitons (wave-corpuscles). Such solutions provide an example for which conditions of Theorem 2.1 hold. We assume a purely electric external EM field, i.e. when $\mathbf{A}_{\text{ex}} = 0$, $\mathbf{E}_{\text{ex}}(t, \mathbf{x}) = -\nabla\varphi_{\text{ex}}(t, \mathbf{x})$. For the purely electric external field the field equations (30), (31) take the form (72). We define the *wave-corpuscle* ψ, φ by the following formula:

$$\begin{aligned} \psi(t, \mathbf{x}) &= e^{iS/\chi} \hat{\psi}, \quad S = m\mathbf{v} \cdot (\mathbf{x} - \mathbf{r}) + s_p(t), \\ \hat{\psi} &= \dot{\psi}(|\mathbf{x} - \mathbf{r}|), \quad \varphi = \dot{\varphi}(|\mathbf{x} - \mathbf{r}|), \quad \mathbf{r} = \mathbf{r}(t). \end{aligned} \quad (94)$$

In the above formula $\dot{\psi}$ is the form factor satisfying (35), $\dot{\varphi}$ is a radial function determined from (31).

We refer to the function $\mathbf{r}(t)$ as wave-corpuscle center. Since $\hat{\psi}$ is center-symmetric, this definition agrees with more general definition (58). Note that in a simpler case when the external fields φ_{ex} and \mathbf{A}_{ex} vanish, a simpler solution of (72) and (83) is provided by (94) with $\mathbf{r}(t) = \mathbf{r}_0 + \mathbf{v}t$ with a constant velocity \mathbf{v} . In this case the wave-corpuscle solution (94) of the field equations (72)-(73) can be obtained from the rest solution $\dot{\psi}, \dot{\varphi}$ by certain Galilean-gauge transformations. Solutions of a similar form are known in the theory of nonlinear Schrödinger equations, see [36] and references therein. For the particular case of the logarithmic nonlinearity solutions of the form (94) were found in [12] in the form of accelerating gaussions.

Theorem 2.3. *Suppose that $\varphi_{\text{ex}}(t, \mathbf{x})$ is a continuous function which is linear with respect to \mathbf{x} . Then ψ defined by (94) is an exact solution to (72), provided that $\mathbf{r}(t)$ is determined from the equation*

$$m \frac{d^2\mathbf{r}(t)}{dt^2} = q\mathbf{E}_{\text{ex}}(t, \mathbf{r}), \quad (95)$$

and $\mathbf{v}(t), s_p(t)$ are determined by formulas

$$\mathbf{v} = \frac{d\mathbf{r}}{dt}, \quad s_p = \int_0^t \left(\frac{m\mathbf{v}^2}{2} - q\varphi_{\text{ex}}(t, \mathbf{r}(t)) \right) dt'. \quad (96)$$

Proof. If the potential $\varphi_{\text{ex}}(t, \mathbf{x})$ is linear in \mathbf{x} then for any given trajectory $\mathbf{r}(t)$ we can write

$$\varphi_{\text{ex}}(t, \mathbf{x}) = \varphi_{0,\text{ex}}(t) + \varphi'_{0,\text{ex}}(t) \cdot (\mathbf{x} - \mathbf{r}(t)), \quad (97)$$

where

$$\varphi'_{0,\text{ex}}(t) = \nabla_{\mathbf{x}}\varphi_{\text{ex}}(\mathbf{r}(t), t), \quad \varphi_{0,\text{ex}}(t) = \varphi_{\text{ex}}(t, \mathbf{r}(t)).$$

Observe that the representation (94) implies

$$\partial_t \psi = \exp\left(i\frac{S}{\chi}\right) \left\{ \left[\frac{im}{\chi} (\dot{\mathbf{v}} \cdot (\mathbf{x} - \mathbf{r}) - \mathbf{v} \cdot \dot{\mathbf{r}}) + \frac{is_p}{\chi} \right] \hat{\psi} - \dot{\mathbf{r}} \cdot \nabla \hat{\psi} \right\}, \quad (98)$$

and by Leibnitz formula we have

$$\nabla^2 \psi = \exp\left(i\frac{S}{\chi}\right) \left[\left(\frac{im\mathbf{v}}{\chi} \right)^2 \hat{\psi} + 2 \frac{im}{\chi} \mathbf{v} \cdot \nabla \hat{\psi} + \nabla^2 \hat{\psi} \right]. \quad (99)$$

Substituting the expression (94) into the field equations (72) we obtain the following equation for functions \mathbf{v} , \mathbf{r} , s_p :

$$\begin{aligned} & [-m\dot{\mathbf{v}} \cdot (\mathbf{x} - \mathbf{r}) - \mathbf{v} \cdot \dot{\mathbf{r}} - \dot{s}_p] \hat{\psi} - i\chi \dot{\mathbf{r}} \cdot \nabla \hat{\psi} \\ & - \frac{m}{2} \mathbf{v}^2 \hat{\psi} + i\chi \mathbf{v} \cdot \nabla \hat{\psi} + \frac{\chi^2}{2m} \nabla^2 \hat{\psi} - q\varphi_{\text{ex}} \hat{\psi} - \frac{\chi^2}{2m} G' \hat{\psi} = 0. \end{aligned} \quad (100)$$

Using the charge equilibrium equation (22) we eliminate the nonlinearity G and the Laplacian ∇^2 in the above equation (100) and obtain the following equation equivalent to it:

$$- \left\{ m [\dot{\mathbf{v}} \cdot (\mathbf{x} - \mathbf{r}) - \mathbf{v} \cdot \dot{\mathbf{r}}] + \frac{m}{2} \mathbf{v}^2 + \dot{s}_p + q\varphi_{\text{ex}} \right\} \hat{\psi} - i\chi (\dot{\mathbf{r}} - \mathbf{v}) \nabla \hat{\psi} = 0. \quad (101)$$

Now, we equate to zero the coefficients before $\nabla \hat{\psi}$ and $\hat{\psi}$ in that equation, resulting in two equations:

$$\mathbf{v} = \dot{\mathbf{r}}, \quad m [\dot{\mathbf{v}} \cdot (\mathbf{x} - \mathbf{r}) - \mathbf{v} \cdot \dot{\mathbf{r}}] + \frac{m}{2} \mathbf{v}^2 + \dot{s}_p + q\varphi_{\text{ex}} = 0, \quad (102)$$

where, in view of the representation (97), the second equation in (102) can be recast as

$$m [\dot{\mathbf{v}} \cdot (\mathbf{x} - \mathbf{r}) - \mathbf{v} \cdot \dot{\mathbf{r}}] + \dot{s}_p + \frac{m\mathbf{v}^2}{2} + q [\varphi_{0,\text{ex}} + \varphi'_{0,\text{ex}} \cdot (\mathbf{x} - \mathbf{r})] = 0. \quad (103)$$

Then we equate to zero the coefficient before $(\mathbf{x} - \mathbf{r})$ and the remaining coefficient and obtain the following pair of equations:

$$m\dot{\mathbf{v}} = -q\varphi'_{0,\text{ex}}(t), \quad \dot{s}_p - m\mathbf{v} \cdot \dot{\mathbf{r}} + \frac{m\mathbf{v}^2}{2} + q\varphi_{0,\text{ex}}(t) = 0. \quad (104)$$

Based on the first equation (102) and the equations (104) we conclude that the wave-corpuscle defined by the formula (94) and equations (95), (96) is indeed an exact solution to the field equations (72). \square

Remark 3. The above construction does not depend on the nonlinearity $G' = G'_a$ as long as (22) is satisfied. It is uniform with respect to $a > 0$, and the dependence on a in (94) is only through $\dot{\psi}(|\mathbf{x} - \mathbf{r}|) = a^{-3/2} \dot{\psi}_1(a^{-1} |\mathbf{x} - \mathbf{r}|)$. Obviously, if $\psi(t, \mathbf{x})$ is defined by (94) then $|\psi(t, \mathbf{x})|^2 \rightarrow \delta(\mathbf{x} - \mathbf{r})$ as $a \rightarrow 0$ and condition (82) is fulfilled.

Remark 4. The form (94) of exact solutions constructed in Theorem 2.3 is the same as the WKB ansatz in the quasi-classical approach. The trajectories of the charges centers coincide with trajectories that can be found by applying well-known quasiclassical asymptotics to solutions of (30) if one neglects the nonlinearity. Note though that there are two important effects of the nonlinearity not presented in the standard quasiclassical approach. First of all, due to the nonlinearity the charge preserves its shape in the course of evolution whereas in the linear model any wavepacket disperses over time. Second of all, the quasiclassical asymptotic expansions produce infinite asymptotic series which provide for a formal solution, whereas the properly introduced nonlinearity as in (22), (36) allows one to obtain an exact solution. For a treatment of mathematical aspects of the approach to nonlinear wave mechanics based on the WKB asymptotic expansions we refer the reader to [24] and references therein.

Similarly one can consider a single charge in an external EM field which can have nonzero magnetic component. In this case the wave-corpuscle is again defined by relations (94) but equations (95) are replaced by (83), see [5] for details.

3. MULTIHARMONIC SOLUTIONS FOR A SYSTEM OF MANY CHARGES

In this section we consider a regime of close interaction which models a system of bound charges. This regime differs significantly from the regime of remote interaction considered in Section 2. More specifically, we seek special form solutions to the field equations (30), (31) for which (i) the potentials φ^ℓ are time independent; (ii) every wave functions ψ^ℓ depends on time harmonically through gauge factor $e^{-i\omega_\ell t}$ with possibly different values of frequencies ω_ℓ for different ℓ . We refer to such solutions as multiharmonic. Note that multiharmonic solutions naturally arise in the analysis of nonlinear dispersive equations and systems, see [2].

Let us consider the field equations (30) and (31) without external fields, namely

$$i\chi\partial_t\psi^\ell + \frac{\chi^2}{2m^\ell}\nabla^2\psi^\ell - q^\ell\varphi_{\neq\ell}\psi^\ell = \frac{\chi^2}{2m^\ell}G'_\ell\left(\left|\psi^\ell\right|^2\right)\psi^\ell, \quad \ell = 1, \dots, N, \quad (105)$$

with $\varphi_{\neq\ell}$ defined by (23)

$$\varphi_{\neq\ell} = \sum_{\ell' \neq \ell} \varphi^{\ell'}, \quad \frac{1}{4\pi}\nabla^2\varphi^{\ell'} = -q^{\ell'}\left|\psi^{\ell'}\right|^2. \quad (106)$$

The total energy of the system is given by the formula

$$\begin{aligned} \mathcal{E} &= \sum_{\ell} \mathcal{E}_{\ell}, & (107) \\ \mathcal{E}_{\ell} &= \frac{1}{2} \int q^{\ell} \left|\psi^{\ell}\right|^2 \varphi_{\neq\ell} d\mathbf{x} + \int \frac{\chi^2}{2m^{\ell}} \left\{ \left|\nabla\psi^{\ell}\right|^2 + G^{\ell}\left(\left|\psi^{\ell}\right|^2\right) \right\} d\mathbf{x}, \end{aligned}$$

where $\varphi_{\neq\ell}$ is defined in (106), $\varphi^{\ell'}$ are given by (32). The energy \mathcal{E} is a conserved quantity for the system (105), (106), it can be derived in a standard way from the Lagrangian (26) taking in account equations (105), (106). Collecting terms in the expression for \mathcal{E} which explicitly involve ψ^{ℓ} with a given ℓ we introduce ℓ -th charge energy in the system's field by the formula

$$\mathsf{E}_{0\ell} = \int q^{\ell} \left|\psi^{\ell}\right|^2 \varphi_{\neq\ell} d\mathbf{x} + \int \frac{\chi^2}{2m^{\ell}} \left\{ \left|\nabla\psi^{\ell}\right|^2 + G^{\ell}\left(\left|\psi^{\ell}\right|^2\right) \right\} d\mathbf{x}. \quad (108)$$

Here and below integrals with respect to spatial variables are over \mathbb{R}^3 . We call so defined $\mathsf{E}_{0\ell}$ the ℓ -th particle energy in system field. Note that for a single particle $\mathsf{E}_{0\ell} = \mathcal{E}_{\ell} = \mathcal{E}$, in the general case $N \geq 2$ the total energy \mathcal{E} does not equal the sum of $\mathsf{E}_{0\ell}$, see for example (144) for the case of two interacting charges; in fact the difference between the sum of $\mathsf{E}_{0\ell}$ and the total energy \mathcal{E} coincides with the total energy of EM fields. In accordance with (53) we assume that $\psi^{\ell} \in \Xi$ where

$$\Xi = \left\{ \psi \in H^1(\mathbb{R}^3) : \|\psi\|^2 = \int |\psi|^2 d\mathbf{x} = 1 \right\}. \quad (109)$$

Theorem 3.1. *Let $G_{\ell}(s)$ be a function of class C^1 which is subcritical, namely there exists $\delta > 0$ and C such that*

$$\left| \int G_{\ell}\left(\left|\psi\right|^2\right) d\mathbf{x} \right| \leq C + C \|\psi\|_{H^1}^{2-\delta} \text{ for all } \psi \in \Xi, \quad \ell = 1, \dots, N. \quad (110)$$

Then the functional \mathcal{E} is bounded from below on the set Ξ^N and boundedness of \mathcal{E} implies boundedness of $\|\psi^\ell\|_{H^1}$, $\ell = 1, \dots, N$. Boundedness of \mathcal{E} on Ξ^N is equivalent to boundedness of all $E_{0\ell}$, $\ell = 1, \dots, N$.

Proof. Note that according to (32)

$$\int |\psi^\ell|^2 \varphi^\ell d\mathbf{x} = \int \int |\psi^\ell(\mathbf{x})|^2 \frac{1}{|\mathbf{x} - \mathbf{y}|} |\psi^\ell(\mathbf{y})|^2 d\mathbf{xdy}.$$

Splitting the domain of integration into $|\mathbf{x} - \mathbf{y}| \geq \theta$ and $|\mathbf{x} - \mathbf{y}| < \theta$ with arbitrary small θ and using the Sobolev imbedding theorem we obtain the following inequality

$$\begin{aligned} & \int |\psi^\ell(\mathbf{x})|^2 \frac{1}{|\mathbf{x} - \mathbf{y}|} |\psi^\ell(\mathbf{y})|^2 d\mathbf{xdy} \leq \\ & \leq C_\epsilon \|\psi^\ell\|^2 \|\psi^\ell\|^2 + \epsilon \|\psi^\ell\|_{H^1} \|\psi^\ell\|_{H^1} \|\psi^\ell\| \|\psi^\ell\|, \end{aligned} \quad (111)$$

where ϵ can be chosen arbitrary small. From this inequality and (110) we obtain the statement of the theorem. \square

Let us consider now multiharmonic solutions to the system (105), (106), that is solutions of the form

$$\psi^\ell(t, \mathbf{x}) = e^{-i\omega_\ell t} \psi_\ell(\mathbf{x}), \quad \varphi^\ell(t, \mathbf{x}) = \varphi_\ell(\mathbf{x}). \quad (112)$$

Note that we use lower index for $\psi_\ell(\mathbf{x})$ to differ it from $\psi^\ell(t, \mathbf{x})$. Then the functions $\psi_\ell(\mathbf{x})$ satisfy the following nonlinear eigenvalue problem

$$\chi \omega_\ell \psi_\ell + \frac{\chi^2}{2m^\ell} \nabla^2 \psi_\ell - q^\ell \varphi_{\neq \ell} \psi_\ell - \frac{\chi^2}{2m^\ell} G'_\ell(|\psi_\ell|^2) \psi_\ell = 0, \quad (113)$$

where $\varphi_{\neq \ell}$ is defined by (23), $\ell = 1, \dots, N$.

3.1. Planck-Einstein frequency-energy relation and the logarithmic nonlinearity. The nonlinear eigenvalue problem (113), (106) may have many solutions, and every solution $\{\psi_\ell\}_{\ell=1}^N$ determines a set of frequencies $\{\omega_\ell\}_{\ell=1}^N$ and energies $\{E_{0\ell}\}_{\ell=1}^N$. Recall that the fundamental Planck-Einstein frequency-energy relation reads

$$E = \hbar\omega. \quad (114)$$

We would like to find if possible a nonlinearity having the following property: for any two solutions $\{\psi_\ell\}_{\ell=1}^N$, $\{\psi'_\ell\}_{\ell=1}^N$ with the corresponding frequencies $\{\omega_\ell\}_{\ell=1}^N$, $\{\omega'_\ell\}_{\ell=1}^N$ and energies $\{E_{0\ell}\}_{\ell=1}^N$, $\{E'_{0\ell}\}_{\ell=1}^N$ the following *Planck-Einstein frequency-energy relation* holds:

$$\chi(\omega_\ell - \omega'_\ell) = E_{0\ell} - E'_{0\ell}, \quad \ell = 1, \dots, N. \quad (115)$$

We want the above relation (115) to hold for any regular multiharmonic solution of a system of the form (113), (106). Let us consider first the frequencies ω_ℓ which can be determined from the equations as follows. Multiplying the ℓ -th equation (113) by ψ_ℓ^* , integrating the result with respect to the space variable and using the charge normalization condition we obtain

$$\chi \omega_\ell = \int \left[\frac{\chi^2}{2m^\ell} |\nabla \psi_\ell|^2 d\mathbf{y} + q^\ell \varphi_{\neq \ell} |\psi_\ell|^2 \right] d\mathbf{y} + \int \frac{\chi^2}{2m^\ell} G'_\ell(|\psi_\ell|^2) |\psi_\ell|^2 d\mathbf{y}. \quad (116)$$

Comparing the above with (108) we see that

$$\chi \omega_\ell - E_{0\ell} = \frac{\chi^2}{2m^\ell} \int \left[G'_\ell(|\psi_\ell|^2) |\psi_\ell|^2 - G_\ell(|\psi_\ell|^2) \right] d\mathbf{y}. \quad (117)$$

For two solutions $\{\psi_\ell\}_{\ell=1}^N, \{\psi'_\ell\}_{\ell=1}^N$ we obtain the following relations linking their frequencies and energies to the nonlinearities:

$$\begin{aligned} & \chi(\omega_\ell - \omega'_\ell) - (\mathsf{E}_{0\ell} - \mathsf{E}'_{0\ell}) = \\ & = \frac{\chi^2}{2m^\ell} \int G_\ell(|\psi'_\ell|^2) - G'_\ell(|\psi'_\ell|^2) |\psi'_\ell|^2 \, dy - \\ & - \frac{\chi^2}{2m^\ell} \int G_\ell(|\psi_\ell|^2) - G'_\ell(|\psi_\ell|^2) |\psi_\ell|^2 \, dy. \end{aligned} \quad (118)$$

To find a sufficient condition for (115) to hold, we take into account the charge normalization condition $\|\psi_\ell\| = 1$ and observe that it is sufficient to impose the following condition

$$\int [G_\ell(|\psi_\ell|^2) - G'_\ell(|\psi_\ell|^2) |\psi_\ell|^2] \, dy = \text{const} \quad (119)$$

for every $|\psi_\ell|^2$ with $\|\psi_\ell\| = 1$, where the constant may depend on ℓ . This condition is fulfilled if the following differential equation with independent variable $s = |\psi|^2$ holds:

$$s \frac{d}{ds} G_\ell(s) - G_\ell(s) = K_G s \quad (120)$$

with K_G that depends only on ℓ . Then (117) and the normalization condition imply

$$\chi \omega_\ell - \mathsf{E}_{0\ell} = \frac{\chi^2}{2m^\ell} \int [G'_\ell(|\psi_\ell|^2) |\psi_\ell|^2 - G_\ell(|\psi_\ell|^2)] \, dy = -\frac{\chi^2}{2m^\ell} K_G \quad (121)$$

and hence (115) is fulfilled.

Solving the differential equation (120) we obtain the following explicit formula for the *logarithmic nonlinearity*

$$G_\ell(s) = K_G s \ln s + Cs.$$

Comparing with (50) and (49) we find that *if $K_G < 0$ this is exactly the nonlinearity (50) which corresponds to the Gaussian factor*. According to (49) the above formula takes the form

$$G_\ell(s) = G_{\ell,a}(s) = -\frac{1}{(a^\ell)^2} s \ln s + \frac{1}{(a^\ell)^2} s \left(\ln \frac{1}{\pi^{3/2}} - 2 - 3 \ln a \right)$$

where a^ℓ is the size parameter for ℓ -th charge. If $K_G = 0$ then $G_\ell(|\psi_\ell|^2)$ is quadratic and equation (113) turns into the linear Schrödinger equation for which fulfillment of the Planck-Einstein relation is a well-known fundamental property. It is absolutely remarkable that the logarithmic nonlinearity which is singled out by the fulfillment of the Planck-Einstein relation has a second crucial property, namely it allows a localized soliton solution, namely the Gaussian one in (47). Note that above argument can be repeated literally if equation (113) involves external time-independent electric field as in (30), in this case $\varphi_{\neq\ell}$ in the definition (108) of $\mathsf{E}_{0\ell}$ has to be replaced by $\varphi_{\neq\ell} + \varphi_{\text{ex}}$.

Let us study in more detail the situation with the logarithmic nonlinearity singled out by the Planck-Einstein relation. Formula (121) for the Gaussian wave function takes the form

$$\mathsf{E}_{0\ell} = \chi \omega_\ell + \frac{\chi^2}{2(a^\ell)^2 m^\ell}. \quad (122)$$

Theorem 3.2. *Let every $G_\ell(s)$, $\ell = 1, \dots, N$, be the logarithmic function with the derivative defined by (50) with $a = a^\ell$. Then the functional \mathcal{E} defined by (107) is bounded from below on the set Ξ^N . The boundedness of \mathcal{E} or boundedness of all $\{\mathsf{E}_{0\ell}\}_{\ell=1}^N$ implies the boundedness of $\|\psi_\ell\|_{H^1}$ and $\|\psi_\ell\|_X$, where the space X is defined by (137), for every component of $\{\psi_\ell\}_{\ell=1}^N$.*

Proof. The proof of the boundedness from below is similar to the proof of Theorem 3.1: we use (111), and instead of (110) we use (128). From the boundedness of \mathcal{E} or $\{\mathsf{E}_{0\ell}\}_{\ell=1}^N$ and (128) we infer the boundedness in H^1 , and from the boundedness of $\int G_\ell(|\psi_\ell|^2) \, d\mathbf{x}$ we infer the boundedness of $\|\psi_\ell\|_X$. \square

Theorem 3.3. *Let $G_\ell(s)$, $\ell = 1, \dots, N$ be the logarithmic functions with derivatives defined by (50) with $a = a^\ell$. Assume that we have a set of solutions $\{\psi_\ell^\sigma\}_{\ell=1}^N \in \Xi^N$, $\sigma \in \Sigma$ of the nonlinear eigenvalue problem (113), (106) with the corresponding frequencies $\{\omega_\ell^\sigma\}_{\ell=1}^N$ and finite energies $\{\mathsf{E}_{0\ell}^\sigma\}_{\ell=1}^N$. Then for any two solutions $\psi_\ell^\sigma = \psi_\ell$ and $\psi_\ell^{\sigma_1} = \psi_\ell'$ with $\sigma, \sigma_1 \in \Sigma$ the Planck-Einstein relation (115) is fulfilled.*

Proof. According to Theorem 3.2 the boundedness of $\mathsf{E}_{0\ell}^\sigma$ for every given σ implies that functions ψ_ℓ^σ are bounded in H^1 and in X . Let us consider the left-hand side of (113) and denote it by $F(\psi_\ell)$. Similarly to (111) we obtain that

$$\left| \int \psi_\ell f \varphi_{\ell'} \, d\mathbf{x} \right| \leq C \|\psi_\ell\|_{H^1} \|f\|_{H^1},$$

where C does not depend on f . Hence multiplication by $\varphi_{\ell'}$ is a bounded operator from H^1 to H^{-1} . Using this fact to obtain continuous dependence of the term $\varphi_{\neq\ell} \psi_\ell$ on ψ_ℓ and using Lemma 9.3.3 in [15] for remaining terms in $F(\psi_\ell)$, we conclude that the functional $F(\psi_\ell)$ depends continuously in space W^* defined in (138) on $\psi_\ell \in H^1 \cap X$ and it is bounded in W^* . Since

$$\int F(\psi_\ell) \psi_\ell \, d\mathbf{x} = \chi \omega_\ell \int |\psi_\ell|^2 \, d\mathbf{x} - \mathsf{E}_{0\ell} + \frac{\chi^2}{2(a^\ell)^2 m^\ell} \int |\psi_\ell|^2 \, d\mathbf{x}$$

(117) holds for smooth rapidly decaying functions ψ_ℓ , we can use in a standard way that smooth functions with compact support are dense in $H^1 \cap X$ and obtain (117) written in the form

$$\chi \omega_\ell^\sigma - \mathsf{E}_{0\ell}^\sigma = -\frac{\chi^2}{2(a^\ell)^2 m^\ell} \int |\psi_\ell^\sigma|^2 \, d\mathbf{x}$$

for functions ψ_ℓ^σ from $H^1 \cap X$. The right-hand side does not depend on σ thanks to the normalization condition (53), and we obtain (115). \square

We would like to stress remarkable universality of the Planck-Einstein relation (115) proven above for multiharmonic solutions and the fact that it holds for every individual particle in a system of many interacting particles. Namely, the Planck-Einstein relation holds with the same coefficient χ for an arbitrary pair of solutions of (113), (106) and for an arbitrary component of those solutions, and the validity of this relation does not depend on the number N which equals the number of interacting particles. Observe also that the derivation of (121) and (122) is based only on properties of the nonlinear terms as in (118) and can be extended to more general systems than (105), (106). In particular, the systems may involve linear terms with potentials which explicitly depend on x as in (172).

The connection between the logarithmic nonlinearity and the Planck-Einstein frequency-energy relation was discovered in a different setting by Bialynicki-Birula and Mycielski in [12]. Note though that in [12] a system of N particles is described as in the quantum mechanics by a single wave function ψ over $3N$ -dimensional configuration space, whereas in our model every of N particles has its own wave function ψ_ℓ depending on 3 spatial variables. This is why our approach naturally leads to the study of *multi-harmonic solutions* for interacting particles for which every individual wave function ψ_ℓ can be associated with its individual frequency ω_ℓ . Another significant difference between our approach and the nonlinear mechanics in [12] is the way the nonlinearity enters the Lagrangian and the field equations for $N \geq 2$ particles. Namely, in our approach every individual particle has its own nonlinearity whereas in [12] there is a single nonlinearity for the entire system of N particles.

3.2. Gaussian shape as a global minimum of energy. As one can see from the previous section the logarithmic nonlinearity defined by (48) is singled out by the requirement that the Planck-Einstein frequency-energy relation holds exactly. Let us look further into the properties of the logarithmic nonlinearity.

We already observed that the equilibrium equation with the logarithmic nonlinearity admits the Gaussian function as an exact solution. This solution is a critical point of the energy, and we show below that the Gaussian function provides a unique (modulo translations) minimum of the energy functional on functions subjected to the charge normalization condition. This fact was already found in [12].

Let us consider the energy $\mathcal{E}(\psi) = E_0(\psi)$ restricted to one particle with $\varphi_{\text{ex}} = 0$ and G^ℓ defined for $a = 1$ by (49), namely

$$\mathcal{E}(\psi) = \frac{\chi^2}{2m^\ell} \int \left\{ |\nabla \psi|^2 - |\psi|^2 \ln |\psi|^2 + |\psi|^2 \left(\ln \frac{1}{\pi^{3/2}} - 2 \right) \right\} d\mathbf{x}. \quad (123)$$

Of course, the case $a > 0$ can be considered similarly. We consider this functional on a set Ξ defined by (109). In the following theorem we show based on the logarithmic Sobolev inequality that the Gaussian function $\psi_g = C_g e^{-|\mathbf{x}|^2/2}$ provides the global minimum of the energy, and that all the global minima belong to the set

$$\Omega = \{ \psi : \psi = e^{i\theta} \psi_g(\cdot - \mathbf{r}), \quad \mathbf{r} \in \mathbb{R}^3, \quad \theta \in \mathbb{R} \} \quad (124)$$

obtained from ψ_g by spatial translations and gauge factor multiplication. Another proof of this statement is given in [14].

Theorem 3.4. *Let $\psi \in \Xi$. Then, if $a = 1$*

$$\mathcal{E}(\psi) \geq \mathcal{E}(\psi_g) = \frac{\chi^2}{2m^\ell} \quad (125)$$

and the equality holds only for $\psi \in \Omega$.

Proof. For simplicity we set here $\frac{\chi^2}{m^\ell} = 1$. The value of the energy $\mathcal{E}(\psi)$ on ψ_g can be found explicitly:

$$\mathcal{E}(\psi_g) = \frac{1}{2}. \quad (126)$$

Note that the Euler equation for constrained critical points of $\mathcal{E}(\psi)$ has the form

$$\lambda\psi + \nabla^2\psi = \left(-\ln(|\psi|^2) + \left(\ln \frac{1}{\pi^{3/2}} - 3 \right) \right) \psi, \quad (127)$$

and ψ_g satisfies this equation. Now we show that ψ_g provides the global minimum of $\mathcal{E}(\psi)$ defined by (123) for real-valued ψ . We will use the following Euclidean logarithmic Sobolev inequality

$$\int_{\mathbb{R}^d} \psi^2 \ln \psi^2 \, d\mathbf{x} \leq \frac{d}{2} \ln \left[\frac{2}{\pi d e} \int_{\mathbb{R}^d} |\nabla \psi|^2 \, d\mathbf{x} \right] \quad (128)$$

for functions from $H^1(\mathbb{R}^d)$ where equality holds only for Gaussian functions (see [11]). Therefore,

$$\begin{aligned} \mathcal{E}(\psi) &\geq & (129) \\ \frac{1}{2} \left\{ \int \left[|\nabla \psi|^2 + |\psi|^2 \left(\ln \frac{1}{\pi^{3/2}} - 2 \right) \right] \, d\mathbf{x} - \frac{3}{2} \ln \left[\frac{2}{3\pi e} \int_{\mathbb{R}^d} |\nabla \psi|^2 \, d\mathbf{x} \right] \right\} \\ &= \frac{1}{2} \left\{ \int |\nabla \psi|^2 \, d\mathbf{x} - \frac{1}{2} - \frac{3}{2} \ln \left[\frac{2}{3} \int_{\mathbb{R}^d} |\nabla \psi|^2 \, d\mathbf{x} \right] \right\}. \end{aligned}$$

To find $\int_{\mathbb{R}^d} |\nabla \psi|^2 \, d\mathbf{x}$ we consider the Euler equation (127) for the minimizer ψ . From Pohozaev identity applied to (127) we obtain:

$$\frac{1}{2} \int \frac{1}{2} G(|\Psi|^2) \, d\mathbf{x} = \lambda \|\psi\|^2 - \frac{1}{6} \int |\nabla \Psi|^2 \, d\mathbf{x}, \quad (130)$$

where

$$G(|\psi|^2) = -|\psi|^2 \ln |\psi|^2 + |\psi|^2 \left(\ln \frac{1}{\pi^{3/2}} - 2 \right).$$

Multiplying equation (127) by ψ and integrating the result we get

$$\lambda \|\psi\|^2 - \mathcal{E}(\psi) = -\frac{1}{2} \int |\psi|^2 \, d\mathbf{x} = -\frac{1}{2}. \quad (131)$$

Adding (130) and (131) we obtain

$$-\frac{\chi^2}{2m^\ell} \int |\nabla \psi|^2 \, d\mathbf{x} = -\frac{1}{2} - \frac{1}{6} \int |\nabla \Psi|^2 \, d\mathbf{x},$$

and hence

$$\int |\nabla \psi|^2 \, d\mathbf{x} = \frac{3}{2}.$$

Substitution of the above expression into inequality (129) implies $\mathcal{E}(\psi) \geq \frac{1}{2}$ where the equality holds only for Gaussian functions. Since ψ is a minimizer, the inequality holds for any real $\psi \in \Xi$. Let us consider now a complex minimizer $\psi = u + iv$ such that $\mathcal{E}(\psi) \leq \frac{1}{2}$. Notice that the following elementary inequality holds

$$|\nabla (u^2 + v^2)^{1/2}|^2 \leq |\nabla u|^2 + |\nabla v|^2$$

if $u^2 + v^2 \neq 0$ and the equality is possible only if $v\nabla u = u\nabla v$. The above inequality implies in particular that $(u^2 + v^2)^{1/2} \in H^1$. Applying once more the Euclidean logarithmic Sobolev inequality for real functions we get

$$\frac{1}{2} \geq \mathcal{E}(\psi) \geq \mathcal{E}\left((u^2 + v^2)^{1/2}\right).$$

For such a minimizer $(u^2 + v^2)^{1/2}$ must coincide with a Gaussian function and equality $v\nabla u = u\nabla v$ must hold a.e.. Since

$$\nabla \ln u = \frac{\nabla u}{u} = \frac{\nabla v}{v} = \nabla \ln v$$

for non-zero u and v , we conclude that $\ln u - \ln v$ is a constant and the complex minimizer ψ is obtained from a Gaussian function via multiplication by a gauge factor $e^{i\theta}$. \square

The following theorem directly follows from results of Cazenave and Lions [17].

Theorem 3.5. *Let Ω_ϵ be ϵ -neighborhood in H^1 norm of Ω*

$$\Omega_\epsilon = \left\{ \psi \in \Xi : \inf_{v \in \Omega} \|\psi - v\|_{H^1} \leq \epsilon \right\}, \quad (132)$$

and M_δ be a sublevel set

$$M_\delta = \{ \psi \in \Xi : \mathcal{E}(\psi) \leq \mathcal{E}(\psi_g) + \delta \}. \quad (133)$$

Then for any $\epsilon > 0$ there exists $\delta > 0$ such that $M_\delta \subset \Omega_\epsilon$.

Proof. Assume the contrary, namely that there exists $\epsilon > 0$ and a sequence $\psi_j \in \Xi$ such that $\mathcal{E}(\psi_j) \rightarrow \mathcal{E}(\psi_g)$ and $\inf_{v \in \Omega} \|\psi_j - v\|_{H^1} \geq \epsilon$. According to Theorem II.1 and Remark II.3 in [17] a subsequence $\psi_j(\cdot - \mathbf{r}_j)$ is relatively compact in H^1 . Hence there is a subsequence that converges in H^1 to a global minimizer which belongs to Ω . This contradicts the assumption $\epsilon > 0$. \square

Let us consider now one-particle equation (105) with logarithmic nonlinearity in the absence of external fields (a free particle)

$$i\chi \partial_t \psi = -\frac{\chi^2}{2m} \nabla^2 \psi + \frac{\chi^2}{2m} \left(-\ln(|\psi|^2 / C_g^2) - 3 \right) \psi. \quad (134)$$

The existence and the uniqueness of solutions to the initial value problem for this equation is proven in [16]. Since the logarithm has a singularity at $\psi = 0$, to describe classes of functions for which the problem is well-posed we need to introduce special spaces. Following Cazenave [15] we introduce functions

$$\begin{aligned} A(|\psi|) &= -|\psi|^2 \ln |\psi|^2 \text{ if } 0 \leq |\psi| \leq e^{-3}, \\ A(|\psi|) &= 3|\psi|^2 + 4e^{-3}|\psi| - e^{-3} \text{ if } |\psi| \geq e^{-3}, \end{aligned} \quad (135)$$

$$B(|\psi|) = |\psi|^2 \ln |\psi|^2 + A(|\psi|). \quad (136)$$

So defined A is a *convex* C^1 function which is C^2 for $|\psi| \neq 0$. The function $B(|\psi|)$ vanishes for small $|\psi|$ and $\psi B(|\psi|) / |\psi|^2$ is of class C^1 and satisfies uniform Lipschitz condition. Let A^* be the convex conjugate function of A , it is also convex of class C^1 and positive except at zero. We introduce Banach spaces

$$\begin{aligned} X &= \{ \psi \in L^1(\mathbb{R}^3) : A(|\psi|) \in L^1(\mathbb{R}^3) \}, \\ X' &= \{ \psi \in L^1(\mathbb{R}^3) : A^*(|\psi|) \in L^1(\mathbb{R}^3) \}. \end{aligned} \quad (137)$$

Let

$$W = H^1(\mathbb{R}^3) \cap X, \quad W^* = H^1(\mathbb{R}^3) + X'. \quad (138)$$

Note that M_δ is bounded in W . By Lemma 9.3.2 from [15] the function $\psi \rightarrow \psi \ln |\psi|^2$ is continuous from X to X' and is bounded on bounded sets.

According to Cazenave [14], [15], if $\psi_0 \in W$ there exists unique solution $\psi \in C(\mathbb{R}, W) \cap C^1(\mathbb{R}, W^*)$ of (134) with initial data $\psi(0) = \psi_0$. Properties of solutions of (134) are described in [14], [15], in particular $\Xi \cap W$ and M_δ are invariant sets. According to [17] the solution ψ_g is *orbitally stable*, namely invariance of M_δ and Theorem 3.5 imply that if $\psi(0, \cdot) \in M_\delta$ then $\psi(0, t) \in \Omega_\epsilon$ for $t \geq 0$. Consequently, small initial perturbations of the Gaussian shape do not cause its large perturbations

in the course of time evolution given by (134) but may cause considerable spatial shifts of the entire wave function. Such a time evolution of charges in electric field is described in Theorem 2.1. Note that if the potential $\varphi_{\text{ex}}(t, x)$ is linear as in Theorem 2.3, one can rewrite equation (72) in a moving frame with origin $\mathbf{r}(t)$ and corresponding phase correction for ψ as in (94) (see [5] for details) and obtain an equivalent equation of the form (72) with $\varphi_{\text{ex}}(t, \mathbf{x}) = 0$, namely (134). Wave-corpuscle solution (94) after the change of variables turns into ψ_g . Therefore, using Theorem 3.5 we conclude that the wave-corpuscle solutions of (72) constructed in Theorem 2.3 are orbitally stable.

4. TWO PARTICLE HYDROGEN-LIKE SYSTEM

In this section we consider a particular case of multiharmonic solutions of the system (113) with $N = 2$ which models a bound proton-electron system. For this system we discuss general properties and provide a heuristic analysis of the coupling between proton and electron. Using this analysis as a motivation, we then write equations and energy functional for one charge (electron) in the Coulomb field of proton. We study this problem in more detail along the lines of [9], [10].

4.1. Electron-proton system. To model states of a bound proton-electron system, the hydrogen atom, we consider the multiharmonic solutions of (30), (31) described by the system (113), (106) with $N = 2$, where indices ℓ take two values $\ell = 1$ and $\ell = 2$. The charges have opposite values $q_1 = -q_2 = -q$. For brevity we introduce notation

$$\Phi_1 = \varphi_1/q_1, \quad \Phi_2 = \varphi_2/q_2, \quad (139)$$

$$a_1 = \frac{\chi^2}{q^2 m_1}, \quad a_2 = \frac{\chi^2}{q^2 m_2}. \quad (140)$$

The quantity a_1 turns into *the Bohr radius* if χ coincides with Planck constant \hbar , and m_1, q are the electron mass and charge respectively. Using the above notation we rewrite the two-particle system (113), (106) in the form of the following *nonlinear eigenvalue problem*

$$\frac{\chi}{q^2} \omega_1 \psi_1 + \frac{a_1}{2} \nabla^2 \psi_1 + \Phi_2 \psi_1 = \frac{a_1}{2} G'_1 (|\psi_1|^2) \psi_1, \quad (141)$$

$$\frac{\chi}{q^2} \omega_2 \psi_2 + \frac{a_2}{2} \nabla^2 \psi_2 + \Phi_1 \psi_2 = \frac{a_2}{2} G'_2 (|\psi_2|^2) \psi_2, \quad (142)$$

$$\nabla^2 \Phi_1 = -4\pi |\psi_1|^2, \quad \nabla^2 \Phi_2 = -4\pi |\psi_2|^2. \quad (143)$$

The functions ψ_1 and ψ_2 are respectively the wave functions for the electron and the proton. As always, we look for solutions $\psi_\ell \in \Xi$ with Ξ defined by (109). The nonlinearities G'_1, G'_2 are assumed to be logarithmic as defined by (50) where the size parameter $a = a^\ell$ is different for electron and proton. One can similarly consider other nonlinearities but in this paper we stay with the logarithmic ones.

In accordance with (107) we introduce the energy functional by the following formula

$$\begin{aligned} & \mathcal{E}(\psi_1, \psi_2) \\ &= q^2 \int \left[\frac{a_1}{2} |\nabla \psi_1|^2 + \frac{a_1}{2} G_1 (|\psi_1|^2) - 4\pi |\psi_1|^2 (-\nabla^2)^{-1} |\psi_2|^2 \right] d\mathbf{x} \\ & \quad + q^2 \int \left[\frac{a_2}{2} |\nabla \psi_2|^2 + \frac{a_2}{2} G_2 (|\psi_2|^2) \right] d\mathbf{x}, \end{aligned} \quad (144)$$

where $(-\nabla^2)^{-1} |\psi_\ell|^2$ is defined by (32). Equations (141), (142), (143) can be derived from the Euler equations for a critical point of $\mathcal{E}(\psi_1, \psi_2)$ with the constraint $(\psi_1, \psi_2) \in \Xi^2$, if we set in (143) $\Phi_2 = 4\pi \left[(-\nabla^2)^{-1} |\psi_2|^2 \right]$, $\Phi_1 = 4\pi \left((-\nabla^2)^{-1} |\psi_1|^2 \right)$, the frequencies ω_1, ω_2 being proportional to the Lagrange multipliers. Using (32) one can see that

$$\int |\psi_1|^2 (-\nabla^2)^{-1} |\psi_2|^2 d\mathbf{x} = \int |\psi_2|^2 (-\nabla^2)^{-1} |\psi_1|^2 d\mathbf{x}$$

hence the coupling term in (144) is symmetric with respect to ψ_1, ψ_2 . Note also that the first term in formula (144) coincides with the energy E_{01} of the first charge in the system field as given by (108) with $\ell = 1$, and the second term with the expression for the energy $\mathcal{E}_2(\psi_2)$ of a free second particle given by (123). Obviously, $\mathcal{E}(\psi_1, \psi_2)$ also can be written as a sum of energy E_{02} of the second charge in the system field plus the free energy of the first charge.

According to Theorem 3.2 the energy $\mathcal{E}(\psi_1, \psi_2)$ is bounded from below.

Remark 5. Note that system (141)-(143) is similar to the Hartree equations studied in [27], though it differs from it because of the presence of the nonlinearities G_ℓ .

4.2. Reduction to one charge in the Coulomb field. In this subsection we give a motivation for replacing the problem of determination of critical values of the energy functional \mathcal{E} given by (144) for a system of two charges by a simpler problem for a single charge similarly to the Born-Oppenheimer approximation in quantum mechanics. To this end we use two changes of variables in two equations, $\mathbf{x} = a_1 \mathbf{y}_1$ in (141) and $\mathbf{x} = a_2 \mathbf{y}_2$ in (142), where a_ℓ are defined by (140), namely

$$\mathbf{x} = a_\ell \mathbf{y}_\ell, \quad \ell = 1, 2, \quad (145)$$

and rescale the fields as follows:

$$\Phi_\ell(\mathbf{x}) = \frac{\phi_\ell(\mathbf{y}_\ell)}{a_\ell}, \quad \psi_\ell(\mathbf{x}) = \frac{1}{a_\ell^{3/2}} \Psi_\ell(\mathbf{y}_\ell), \quad \ell = 1, 2. \quad (146)$$

Hence (141), (142) takes the form of the following *nonlinear hydrogen system*

$$\frac{\chi}{q^2} \omega_1 \Psi_1 + \frac{1}{2a_1} \nabla_{\mathbf{y}_1}^2 \Psi_1 + \frac{1}{a_2} \phi_2 \left(\frac{a_1}{a_2} \mathbf{y}_1 \right) \Psi_1 = \frac{1}{2a_1} G'_1 \left(|\Psi_1|^2 \right) \Psi_1, \quad (147)$$

$$\frac{\chi}{q^2} \omega_2 \Psi_2 + \frac{1}{2a_2} \nabla_{\mathbf{y}_2}^2 \Psi_2 + \frac{1}{a_1} \phi_1 \left(\frac{a_2}{a_1} \mathbf{y}_2 \right) \Psi_2 = \frac{1}{2a_2} G'_2 \left(|\Psi_2|^2 \right) \Psi_2, \quad (148)$$

$$\nabla_{\mathbf{y}_1}^2 \phi_1 = -4\pi |\Psi_1|^2, \quad \nabla_{\mathbf{y}_2}^2 \phi_2 = -4\pi |\Psi_2|^2. \quad (149)$$

Here we use the same letter G to determine the function of rescaled variables. Note that the electron/proton mass ratio $\frac{m_1}{m_2} \simeq \frac{1}{1837}$ is small, therefore the parameter

$$b = \frac{a_2}{a_1} = \frac{m_1}{m_2} \ll 1 \quad (150)$$

is small too. We rewrite (147), (148) as follows:

$$\frac{\chi a_1}{q^2} \omega_1 \Psi_1 + \frac{1}{2} \nabla^2 \Psi_1 + \frac{1}{b} \phi_2 \left(\frac{\mathbf{y}}{b} \right) \Psi_1 = \frac{1}{2} G'_1 \left(|\Psi_1|^2 \right) \Psi_1, \quad (151)$$

$$\frac{\chi a_2}{q^2} \omega_2 \Psi_2 + \frac{1}{2} \nabla^2 \Psi_2 + b \phi_1 \left(b \mathbf{y} \right) \Psi_2 = \frac{1}{2} G'_2 \left(|\Psi_2|^2 \right) \Psi_2. \quad (152)$$

We would like to show that if we are interested in electron frequencies ω_1 which correspond to lower energy levels of $\mathcal{E}(\psi_1, \psi_2)$ then, in the case $b \rightarrow 0$, it is reasonable to replace system (151), (152) by one equation with the Coulomb potential.

The discrete spectrum of the classical linear non-relativistic Schrödinger operator for hydrogen atom with the Coulomb potential can be recovered (if multiplicities are not taken into account) from radial eigenfunctions. Therefore here we restrict ourselves to the radial solutions of (151), (152) and restrict (144) to radial functions. Consider a radial solution (Ψ_1, Ψ_2) of (151), (152). Equation for the electron frequency ω_1 given by (116) with $\ell = 1$ takes the form

$$\frac{\chi a_1}{q^2} \omega_1 = \int \frac{1}{2} G'_1 \left(|\Psi_1|^2 \right) |\Psi_1|^2 - \frac{1}{2} |\nabla \Psi_1|^2 - \left(\frac{1}{b} \phi_2 \left(\frac{\mathbf{y}}{b} \right) - \frac{1}{|\mathbf{y}|} \right) |\Psi_1|^2 - \frac{1}{|\mathbf{y}|} |\Psi_1|^2 \, d\mathbf{y} \quad (153)$$

with the proton potential ϕ_2 . Then we would like to replace the potential ϕ_2 in (153) by the Coulomb potential $\frac{1}{|\mathbf{y}|}$ as an approximation. To show that for small b one may expect the resulting perturbation of eigenvalues to be small, we use the following representation for the radial potential $\phi(r) = 4\pi (-\nabla^2)^{-1} |\Psi|^2$:

$$\phi(r) = \frac{1}{r} \left[1 - 4\pi \int_r^\infty (r_1 - r) r_1 |\Psi(r_1)|^2 \, dr_1 \right]. \quad (154)$$

The term which we expect to be small is

$$\begin{aligned} D_{\text{prot}} &= - \int \left(\frac{1}{b} \phi_2 \left(\frac{1}{b} \mathbf{y}_1 \right) - \frac{1}{|\mathbf{y}_1|} \right) |\Psi_1|^2 \, d\mathbf{y}_1 = \\ &= 4\pi \int_0^\infty \frac{4\pi}{r} |\Psi_1(r)|^2 r^2 \int_{r/b}^\infty (r_1 - r/b) r_1 |\Psi_2(r_1)|^2 \, dr_1 \, dr. \end{aligned} \quad (155)$$

Changing the order of integration and using substitution $r/b = r_2$ we obtain

$$\begin{aligned} D_{\text{prot}} &= (4\pi)^2 b^2 \int_0^\infty \int_{r_2}^\infty |\Psi_1(br_2)|^2 r_2 (r_1 - r_2) r_1 |\Psi_2(r_1)|^2 \, dr_1 \, dr_2 \\ &= (4\pi)^2 b^2 \int_0^\infty |\Psi_2(r_1)|^2 r_1 \int_0^{r_1} |\Psi_1(br_2)|^2 r_2 (r_1 - r_2) \, dr_2 \, dr_1. \end{aligned}$$

Hence

$$|D_{\text{prot}}| \leq \frac{(4\pi)^2}{6} b^2 \max_r |\Psi_1(r)|^2 \int_0^\infty |\Psi_2(r_1)|^2 r_1^4 \, dr_1. \quad (156)$$

The right-hand side of (156) involves the variance of Ψ_2 and $\|\Psi_1\|_{L^\infty}$. To show that $|D_{\text{prot}}|$ is small it is sufficient to show that the variance of Ψ_2 and $\|\Psi_1\|_{L^\infty}$ are bounded uniformly for small b . Note that Ψ_1, Ψ_2 in (156) are not arbitrary radial functions, but special solutions of (151), (152), (149) which correspond to lower critical energy levels of the energy functional $\mathcal{E} = E_{01} + E_{02}$. Dependence of the coupling between (151) and (152) on b comes through the positive potentials $\frac{1}{b} \phi_2 \left(\frac{1}{b} \mathbf{y} \right)$ and $b \phi_1(b \mathbf{y})$ in (151) and (152) respectively, according to (154) these potentials are bounded by $\frac{1}{|\mathbf{y}|}$ uniformly for $b > 0$. Using the uniform boundedness of the potentials and estimate (182) we conclude that energy and H^1 -norms of Ψ_1 and Ψ_2 are bounded uniformly in b . As in the proof of Lemma 5.3 below, we conclude that radial Ψ_1 and Ψ_2 are bounded in L^5 , they also satisfy (210). From boundedness in L^5 we derive that $\frac{1}{|\mathbf{y}|} \Psi_1$ is bounded in $L^{7/4}$ and so does $G'_1 \left(|\Psi_1|^2 \right) \Psi_1$. Note also that since the energy is bounded from below, the negative values of $\omega = \frac{\chi a_1}{q^2} \omega_1$ in (151) which correspond to lower energy levels are bounded. Hence, the term

$$\frac{1}{b} \phi_2 \left(\frac{1}{b} \mathbf{y} \right) \Psi_1 - \frac{1}{2} G'_1 \left(|\Psi_1|^2 \right) \Psi_1 + \omega \Psi_1$$

in (151) is bounded in $L^{7/4}$, therefore the solution Ψ_1 of the elliptic equation (151) belongs to Sobolev space $W^{7/4,2}$ and by Sobolev imbedding is bounded in L^∞ . As for Ψ_2 , from (210) using the comparison argument as in the proof of Lemma 5.8 we derive exponential decay of solutions of the equation (152) for large r uniformly in b and conclude that the variance of Ψ_2 is uniformly bounded for small b . Hence, for such solutions $|D_{\text{prot}}|$ is small for small b . The smallness of b in (156) (recall that $b \simeq \frac{1}{1837}$ for proton-electron system) gives us a motivation to set $b = 0$ in (152) and replace $\frac{1}{b}\phi_2(\frac{1}{b}\mathbf{y})$ by $\frac{1}{|\mathbf{y}|}$ in (151).

So, we replace the problem of finding frequencies ω_1 by formula (153) based on critical points of $\mathcal{E}(\psi_1, \psi_2)$ which correspond to lower energy levels of $\mathcal{E}(\psi_1, \psi_2)$ by the problem of finding critical points, lower critical levels and corresponding frequencies ω_1 (which for the logarithmic nonlinearity are expressed in terms of the critical levels by (122)) for the following energy functional with the Coulomb potential:

$$\mathcal{E}_{\text{Cb}}(\Psi_1) = \frac{q^2}{a_1\chi} \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla \Psi_1|^2 + \frac{1}{2} G_1(|\Psi_1|^2) - \frac{1}{|\mathbf{y}|} |\Psi_1|^2 \right] d\mathbf{y}. \quad (157)$$

This functional involves only Ψ_1 . In quantum mechanics a somewhat similar reduction (in a completely different setting) from proton-electron system to a single equation with the Coulomb potential is made via Born-Oppenheimer approximation. Additional motivation for the reduction is given in Remark 10.

5. VARIATIONAL PROBLEM FOR A CHARGE IN THE COULOMB FIELD

In this section we consider in detail *radial* critical points of the functional $\mathcal{E}_{\text{Cb}}(\Psi_1)$ defined by (157) and establish its basic properties. In this and following section we look for *real solutions* $\Psi = \Psi^*$ and all function spaces involve only real functions. In what follows we explicitly take into account the dependence of the nonlinearity on the size parameter $a = a^1$ (or on related parameter κ), namely

$$\begin{aligned} G'_{/\kappa}(|\Psi|^2) &= \kappa^2 G'_1(\kappa^{-3} |\Psi|^2), \\ G_{/\kappa}(|\Psi|^2) &= \kappa^5 G_1(\kappa^{-3} |\Psi|^2), \quad \kappa = \frac{a_1}{a}, \end{aligned}$$

where, for consistency with the notation (33) where $a = a_1/\kappa$, we use notation $/\kappa$ to denote the dependence of rescaled G on κ . Note that the dependence on a_1 and $a = a^1$ is factored out after the rescaling, and that $G_{/\kappa}$ in the above formula depends only on their ratio κ . We consider the case of small κ , namely

$$\kappa = \frac{a_1}{a} \ll 1, \quad (158)$$

when the electron size parameter a is much larger than the Bohr radius a_1 . To treat technical difficulties related to the singularity of logarithm at zero, together with the logarithmic nonlinearity given by (50) we use a regularized logarithmic nonlinearity defined as follows:

$$G'_{/\kappa, \xi}(|\psi|^2) = -\kappa^2 \ln_{+,\xi} \left(\kappa^{-3} |\psi|^2 / C_g^2 \right) - 3\kappa^2, \quad (159)$$

where $\xi \leq 0$,

$$\ln_{+,\xi}(s) = \max(\ln(s), \xi) \quad \text{for } s > 0, \quad \ln_{+,\xi}(0) = \xi. \quad (160)$$

For $\xi = -\infty$ we set $\ln_{+,-\infty}(s) = \ln(s)$. The function $\ln_{+,\xi}(s)$ with finite ξ is bounded for bounded s and satisfies Lipschitz condition for $s \geq 0$. Obviously,

$$-\ln_{+,\xi}(s) \leq -\ln_{+,\xi'}(s) \quad \text{for } \xi > \xi' \geq -\infty. \quad (161)$$

Now we describe the basic properties of $G'_{/\kappa,\xi}$ and its integral $G_{/\kappa,\xi}$

$$G_{1,\xi}(s) = \int_0^s G'_{1,\xi}(s') ds', \quad G_{/\kappa,\xi}(s) = -\kappa^5 G_{1,\xi}(\kappa^{-3}s). \quad (162)$$

Proposition 5.1. *The function $G_{/\kappa,\xi}$ with $-\infty \leq \xi \leq 0$ can be written in the form*

$$G_{/\kappa,\xi}(s) = -\kappa^2 s \left(\ln_{+,\xi}(\kappa^{-3}s/C_g^2) + 2 + C_g^2 e^{\xi - \ln_{+,\xi} \kappa^{-3}s} \right) \quad (163)$$

where

$$e^{\xi - \ln_{+,\xi} s} \leq \min \left(1, \frac{e^\xi}{s} \right) \leq 1 \quad (164)$$

and satisfies the inequalities

$$G_{/\kappa,\xi}(s) \leq G_{/\kappa,\xi'}(s) \leq G_{/\kappa,-\infty}(s) = -\kappa^2 s \ln(s) - \kappa^2 s (\ln \kappa^{-3}/C_g^2 + 2), \quad (165)$$

for $0 \geq \xi \geq \xi' \geq -\infty$,

$$\left| G_{1,\xi}(|\Psi|^2) - G_{1,-\infty}(|\Psi|^2) \right| \leq C e^{\xi/4} |\Psi|. \quad (166)$$

Proof. Elementary computation shows that for $s \geq C_g^2 e^\xi$

$$G_{1,\xi}(s) = -s \ln(s/C_g^2) - s (C_g^2 e^{\xi - \ln s} + 2) \quad (167)$$

and

$$G_{1,\xi}(s) = -\xi s - 3s \quad \text{for } s \leq e^\xi C_g^2. \quad (168)$$

Hence

$$G_{1,\xi}(s) = -s (\ln_{+,\xi}(s/C_g^2) + 2 + C_g^2 e^{\xi - \ln_{+,\xi} s}) \quad (169)$$

and (163) holds. Using (161) we derive (165) from (162). Obviously

$$G_{1,\xi}(s) - G_{1,-\infty}(s) = -e^\xi \quad \text{for } s \geq e^\xi C_g^2,$$

and hence

$$\left| G_{1,\xi}(|\Psi|^2) - G_{1,-\infty}(|\Psi|^2) \right| \leq e^{\xi/2} |\Psi| / C_g \quad \text{for } |\Psi|^2 \geq e^\xi C_g^2. \quad (170)$$

For $|\Psi|^2 \leq e^\xi C_g^2$

$$\begin{aligned} \left| G_{1,\xi}(|\Psi|^2) - G_{1,-\infty}(|\Psi|^2) \right| &= |\Psi|^2 \left| \left(\xi - \ln |\Psi|^2 / C_g^2 \right) \right| \\ &\leq e^{\xi/4} C_g |\Psi|^{3/2} \left| \ln |\Psi|^2 / C_g^2 \right| \leq C_1 e^{\xi/4} C_g |\Psi|. \end{aligned} \quad (171)$$

From (170) and (171) we obtain (166). \square

The nonlinear eigenvalue problem with the Coulomb potential has the form similar to (151):

$$\omega \Psi + \frac{1}{2} \nabla^2 \Psi + \frac{1}{|\mathbf{x}|} \Psi = \frac{1}{2} G'_{/\kappa,\xi}(|\Psi|^2) \Psi, \quad (172)$$

where the dimensionless spectral parameter $\omega = \omega_{\kappa,\xi}$ is given by the formula

$$\omega = \frac{\chi a_1}{q^2} \omega^1. \quad (173)$$

Note that equation (172) can be obtained as the Euler equation by variation of the energy functional (157) which we write in the form

$$\mathcal{E}_{\kappa,\xi}(\Psi) = \mathcal{E}_0(\Psi) + \mathcal{G}_{\kappa,\xi}(\Psi), \quad (174)$$

where \mathcal{E}_0 is the quadratic energy functional

$$\mathcal{E}_0 = \int \left(\frac{1}{2} |\nabla \Psi|^2 - \frac{1}{|\mathbf{x}|} |\Psi|^2 \right) d\mathbf{x}, \quad (175)$$

and $\mathcal{G}_{\kappa,\xi}$ is the nonlinear functional

$$\mathcal{G}_{\kappa,\xi}(\Psi) = -\frac{\kappa^2}{2} \int \left(\ln_{+,\xi} \left(\kappa^{-3} |\Psi|^2 / C_g^2 \right) + 2 + C_g^2 e^{\xi - \ln_{+,\xi} \kappa^{-3} |\Psi|^2} \right) |\Psi|^2 d\mathbf{x}. \quad (176)$$

As always we assume the charge normalization constraint

$$\|\Psi\|^2 = \int |\Psi|^2 d\mathbf{x} = 1 \quad (177)$$

and denote similarly to (109) the set of radial functions (which depend only on $|\mathbf{x}|$) by

$$\Xi_{\text{rad}} = \left\{ \Psi \in H_{\text{rad}}^1(\mathbb{R}^3) : \|\Psi\|^2 = 1 \right\}. \quad (178)$$

Obviously, for $\Psi \in \Xi \cap X$ where X is defined by (137)

$$\mathcal{G}_\kappa(\Psi) = \mathcal{G}_{\kappa,-\infty}(\Psi) = -\frac{\kappa^2}{2} \int \left(|\Psi|^2 \ln |\Psi|^2 \right) d\mathbf{x} + \frac{\kappa^2}{2} \left(\ln \frac{1}{\pi^{3/2}} - 2 + 3 \ln \kappa \right). \quad (179)$$

The spectral parameter ω is the Lagrange multiplier and it relates with corresponding critical energy levels $E_n^{\kappa,\xi}$ of $\mathcal{E}_{\kappa,\xi}$ on $\Xi \cap X$ by formula (122) which takes the form

$$E_n^{\kappa,\xi} = \omega_{\kappa,\xi,n} + \frac{\kappa^2}{2}. \quad (180)$$

Let us introduce for $\kappa > 0, \xi \leq 0, \Psi \in \mathbb{C}$ the function

$$g_{\kappa,\xi}(\Psi) = G'_{/\kappa,\xi}(|\Psi|^2) \Psi = \left(-\kappa^2 \ln_{+,\xi} \left(\kappa^{-3} |\Psi|^2 / C_g^2 \right) - 3\kappa^2 \right) \Psi. \quad (181)$$

General properties of functional $\mathcal{E}_{\kappa,\xi}(\Psi)$ with regularized logarithm are described in the following statements.

Lemma 5.2. *The functional $\mathcal{E}_{\kappa,\xi}(\Psi)$ defined by (174), (169) and (176) with $-\infty < \xi \leq 0$ on Ξ_{rad} has the following properties: (i) it is bounded from below on Ξ uniformly in ξ . (ii) If $\Psi \in \Xi$, $\kappa \leq 1$ and $\mathcal{E}_{\kappa,\xi}(\Psi) \leq C$ then $\|\Psi\|_{H^1} \leq C'$ where C' depends only on C . (iii) The functional $\mathcal{E}_{\kappa,\xi}(\Psi)$ is of class C^1 with respect to H^1 norm on Ξ_{rad} . (iv)*

$$\mathcal{G}_{\kappa,\xi}(\Psi) \geq \mathcal{G}_{\kappa,0}(\Psi) \geq -C''\kappa^2 (1 + |\ln \kappa|) \text{ if } \|\Psi\|_{H^1} \leq C'.$$

Proof. Boundedness from below follows from (129), (165) and inequality

$$\int_{\mathbb{R}^3} \frac{1}{|\mathbf{x}|} |\Psi|^2 d\mathbf{x} \leq C_0 \|\Psi\| \|\nabla \Psi\|. \quad (182)$$

From boundedness of $\mathcal{E}_{\kappa,\xi}(\Psi)$, (129) and (165) we obtain boundedness of $\|\nabla \Psi\|$ which on Ξ implies boundedness in H^1 . To prove (iii) observe that by (159)

$$g_{\kappa,\xi}(\Psi) = \kappa^2 (-\xi - 3) \Psi + g_{\kappa,\xi}^1(|\Psi|^2)$$

where $g_{\kappa,\xi}^1(|\Psi|^2)$ is identically zero for small $|\Psi|$ and it has less than quadratic growth for $|\Psi| \rightarrow \infty$. According to Theorem A.VI in [9] then $\mathcal{G}_{\kappa,\xi}(\Psi) + \kappa^2(\xi + 3) \|\Psi\|^2$ is of class C^1 , and hence $\mathcal{G}_{\kappa,\xi}(\Psi)$ is of class C^1 too. To obtain (iv) we use (165) and observe that $\mathcal{G}_{\kappa,0}(\Psi)$ can be estimated in terms of $\|\Psi\|_{L^6}$ which, in turn, can be estimated by $\|\Psi\|_{H^1}$. \square

Lemma 5.3. *Let a sequence of radial functions $\Psi_j \in \Xi_{\text{rad}}$ satisfy (183). Then: (i) a subsequence of Ψ_j converges in $L^p(\mathbb{R}^3)$ and almost everywhere to Ψ_∞ if $2 < p < 6$; (ii) the functions $\Psi_j(\mathbf{x}) \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$ uniformly in j .*

Proof. The estimate (183) together with the normalization condition imply the uniform boundedness of Ψ_j in the Sobolev space $H^1(\mathbb{R}^3)$. According to Theorem A.I' of [9], the space of radial functions $H_{\text{rad}}^1(\mathbb{R}^3)$ is compactly imbedded into $L^p(\mathbb{R}^3)$ if $2 < p < 6$. Hence, a subsequence $\Psi_j(\mathbf{x}) \rightarrow \Psi_\infty(\mathbf{x})$ strongly in $L^p(\mathbb{R}^3)$ and almost everywhere. Statement (ii) follows from Radial Lemma A.II in [9]. \square

The functional $\mathcal{E}_{\kappa,\xi}(\Psi)$ with regularized logarithm satisfies the Palais-Smale condition similar to condition (P-S⁺) in [10]:

Theorem 5.4. *Let $\xi > -\infty$. Let a sequence $\Psi_j \in \Xi_{\text{rad}}$ have the following properties:*

$$\mathcal{E}_{\kappa,\xi}(\Psi_j) \leq -\beta, \quad \beta > 0, \quad (183)$$

and

$$F\Psi_j = \omega_j \Psi_j + \frac{1}{2} \nabla^2 \Psi_j + \frac{1}{|\mathbf{x}|} \Psi_j - \frac{1}{2} g_{\kappa,\xi}(\Psi_j) \rightarrow 0 \quad (184)$$

strongly in $H^{-1}(\mathbb{R}^3)$. Then the sequence contains a subsequence which converges strongly in $H_{\text{rad}}^1(\mathbb{R}^3)$.

Proof. The proof is similar to treatment of radial solutions in [9], [27]. We only sketch main steps. Since (182) holds, (183), (165) and (128) imply boundedness of Ψ_j in $H^1(\mathbb{R}^3)$. Using Lemma 5.3 we conclude that we can choose a subsequence such that $\Psi_j \rightarrow \Psi_\infty$ in $L^5(\mathbb{R}^3)$ and $L^{8/3}(\mathbb{R}^3)$, it converges weakly in $H^{-1}(\mathbb{R}^3)$ and almost everywhere in \mathbb{R}^3 . Multiplying (184) by Ψ_j in $L^2(\mathbb{R}^3) = H$ with inner product $\langle \cdot, \cdot \rangle$ we obtain

$$\begin{aligned} \omega_j \langle \Psi_j, \Psi_j \rangle - \frac{1}{2} \langle \nabla \Psi_j, \nabla \Psi_j \rangle - \frac{1}{2} \left\langle \left(G'_{/\kappa,\xi}(|\Psi_j|^2) \right) \Psi_j, \Psi_j \right\rangle \\ = \langle F\Psi_j, \Psi_j \rangle - \left\langle \frac{1}{|\mathbf{x}|} \Psi_j, \Psi_j \right\rangle. \end{aligned} \quad (185)$$

We rewrite (185) in the form

$$\omega_j \langle \Psi_j, \Psi_j \rangle = \langle F\Psi_j, \Psi_j \rangle + \mathcal{E}_{\kappa,\xi}(\Psi_j) - \int G_{/\kappa,\xi}(|\Psi|^2) - G'_{/\kappa,\xi}(|\Psi|^2) |\Psi|^2 \, d\mathbf{x}.$$

Using (164) we obtain for $\Psi \in \Xi_{\text{rad}}$

$$0 < \int G_{/\kappa,\xi}(|\Psi|^2) - G'_{/\kappa,\xi}(|\Psi|^2) |\Psi|^2 \, d\mathbf{x} \leq \frac{\kappa^2}{2}. \quad (186)$$

Since $\langle F\Psi_j, \Psi_j \rangle \rightarrow 0$, (183) and (186) imply that we can choose a subsequence Ψ_j with $\omega_j \rightarrow \omega_\infty$ where $\omega_\infty \leq -\beta$. Multiplying (184) by a smooth test function with compact support and passing to the limit we obtain in standard way that $\Psi_\infty \in H^1(\mathbb{R}^3)$ satisfies (172) with $\omega = \omega_\infty$.

Now we want to prove that $\Psi_\infty \in \Xi$ and convergence in $H_{\text{rad}}^1(\mathbb{R}^3)$ is strong. We rewrite (185) in the form

$$\begin{aligned} \omega_j \langle \Psi_j, \Psi_j \rangle - \frac{1}{2} \langle \nabla \Psi_j, \nabla \Psi_j \rangle - \frac{1}{2} \left\langle \left(G_{/\kappa, \xi} (|\Psi_j|^2) - \kappa^2 \xi \right) \Psi_j, \Psi_j \right\rangle \\ + \kappa^2 \xi \langle \Psi_j, \Psi_j \rangle = \langle F \Psi_j, \Psi_j \rangle - \left\langle \frac{1}{|\mathbf{x}|} \Psi_j, \Psi_j \right\rangle. \end{aligned} \quad (187)$$

We have $\langle F \Psi_j, \Psi_j \rangle \rightarrow 0$,

$$\omega_j \langle \Psi_j, \Psi_j \rangle + \kappa^2 \xi \langle \Psi_j, \Psi_j \rangle = \omega_j + \kappa^2 \xi \rightarrow \omega_\infty + \kappa^2 \xi.$$

Since $G_{/\kappa, \xi} (|\Psi|^2) - \kappa^2 \xi$ is identically zero for small $|\Psi|^2$ and grows slower than $|\Psi|^3$ as $|\Psi| \rightarrow \infty$, and $|\Psi_j|^5$ are converging in $L^1(\mathbb{R}^3)$, we can apply the compactness Lemma of Strauss (see Theorem A.I in [9]) and obtain

$$\left\langle \left(G_{/\kappa, \xi} (|\Psi_j|^2) - \kappa^2 \xi \right) \Psi_j, \Psi_j \right\rangle \rightarrow \left\langle \left(G_{/\kappa, \xi} (|\Psi_\infty|^2) - \kappa^2 \xi \right) \Psi_\infty, \Psi_\infty \right\rangle.$$

Using the Hölder inequality we obtain that the quadratic mapping $\Psi \rightarrow \frac{1}{|\mathbf{x}|} |\Psi|^2$ is continuous from $L^5(\mathbb{R}^3) \cap L^{8/3}(\mathbb{R}^3)$ into $L^1(\mathbb{R}^3)$. Therefore

$$\left\langle \frac{1}{|\mathbf{x}|} \Psi_j, \Psi_j \right\rangle \rightarrow \left\langle \frac{1}{|\mathbf{x}|} \Psi_\infty, \Psi_\infty \right\rangle.$$

We denote

$$M_0 = \liminf_{j \rightarrow \infty} \langle \Psi_j, \Psi_j \rangle = 1, \quad M_1 = \liminf_{j \rightarrow \infty} \langle \nabla \Psi_j, \nabla \Psi_j \rangle.$$

From (187) we obtain passing to the limit

$$\begin{aligned} (\omega_\infty + \kappa^2 \xi) M_0 - \frac{1}{2} M_1 - \frac{1}{2} \left\langle \left(G_{/\kappa, \xi} (|\Psi_\infty|^2) - \kappa^2 \xi \right) \Psi_\infty, \Psi_\infty \right\rangle \\ = - \left\langle \frac{1}{|\mathbf{x}|} \Psi_\infty, \Psi_\infty \right\rangle. \end{aligned} \quad (188)$$

Multiplying (172) with $\omega = \omega_\infty$ by Ψ in H we obtain

$$\begin{aligned} \omega_\infty \langle \Psi_\infty, \Psi_\infty \rangle - \frac{1}{2} \langle \nabla \Psi_\infty, \nabla \Psi_\infty \rangle - \frac{1}{2} \left\langle \left(G_{/\kappa, \xi} (|\Psi_\infty|^2) - \kappa^2 \xi \right) \Psi_\infty, \Psi_\infty \right\rangle \\ + \kappa^2 \xi \langle \Psi_\infty, \Psi_\infty \rangle = \langle F \Psi_\infty, \Psi_\infty \rangle - \left\langle \frac{1}{|\mathbf{x}|} \Psi_\infty, \Psi_\infty \right\rangle. \end{aligned}$$

Comparing with (188) we obtain

$$(\omega_\infty + \kappa^2 \xi) M_0 - \frac{1}{2} M_1 = (\omega_\infty + \kappa^2 \xi) \langle \Psi_\infty, \Psi_\infty \rangle - \frac{1}{2} \langle \nabla \Psi_\infty, \nabla \Psi_\infty \rangle. \quad (189)$$

From weak convergence in $H_{\text{rad}}^1(\mathbb{R}^3)$ we infer that $M_0 \geq \|\Psi_\infty\|^2$, $M_1 \geq \|\nabla \Psi_\infty\|^2$. Since $(\omega_\infty + \kappa^2 \xi) < 0$, (189) is possible only if $M_0 = \|\Psi_\infty\|^2$, $M_1 = \|\nabla \Psi_\infty\|^2$. These equalities imply that the weak convergence of the subsequence in H^1 to Ψ_∞ is strong. \square

5.1. Nonlinear eigenvalues for a charge in the Coulomb field. In this section we prove that if κ is small enough, the nonlinear eigenvalue problem (172) with logarithmic nonlinearity has solutions with eigenvalues which are close to the eigenvalues of the corresponding linear problem. We look for *real-valued* solutions. As a first step we prove existence of such solutions of the problem with regularized logarithm $\ln_{+, \xi}$. As the second step we pass to the limit as $\xi \rightarrow -\infty$ and obtain solutions of the eigenvalue problem with the original logarithmic nonlinearity.

Consider the linear Schrödinger operator \mathcal{O} with the Coulomb potential which corresponds to $\mathcal{E}_0(\Psi)$, that is

$$\mathcal{O}\Psi = -\frac{1}{2}\nabla^2\Psi - \frac{1}{|\mathbf{x}|}\Psi. \quad (190)$$

Note that \mathcal{O} has the following well known negative eigenvalues

$$E_n^0 = \omega_{0,n} = -\frac{1}{2n^2}, \quad n = 1, 2, \dots \quad (191)$$

which coincide with the negative eigenvalues of the operator \mathcal{O}_{rad} obtained by restriction of \mathcal{O} to radial functions (without counting their multiplicity) and are equal to the negative critical energy levels of $\mathcal{E}_0(\Psi)$. Every eigenvalue of the radial problem

$$\mathcal{O}_{\text{rad}}\Psi_n^0 = \omega_{0,n}\Psi_n^0$$

is simple and corresponding eigenfunctions $\Psi_n^0(r)$ given by well-known explicit formulas decay exponentially as $r \rightarrow \infty$, for example the linear ground state is given by the formula

$$\Psi_1^0(\mathbf{x}) = \frac{1}{\pi^{1/2}}e^{-|\mathbf{x}|}, \quad E_1^0 = -\frac{1}{2}.$$

Let us denote by L_n^0 an eigenspace of \mathcal{O}_{rad} which corresponds to the eigenvalue E_n^0 and consists of radial functions, by $L_n^- \subset H_{\text{rad}}^1$ a finite-dimensional invariant subspace of \mathcal{O}_{rad} which corresponds to eigenvalues $\lambda \leq E_n^0$ and by $L_n^+ \subset H_{\text{rad}}^1(\mathbb{R}^3)$ invariant infinite-dimensional subspace in $H_{\text{rad}}^1(\mathbb{R}^3)$ of \mathcal{O}_{rad} which is orthogonal in L^2 to L_n^- . We have an orthogonal decomposition

$$H_{\text{rad}}^1(\mathbb{R}^3) = L_n^- + L_n^+ = L_{n-1}^- + L_n^0 + L_n^+.$$

We look for eigenvalues $\omega = \omega_{\kappa, \xi, n} < 0$ of the nonlinear eigenvalue problem (172) which can be considered as a perturbation of the eigenvalues E_n^0 . The ground state of $\mathcal{E}_{\kappa, -\infty}(\Psi)$ and the corresponding energy level $\omega_{\kappa, -\infty, 1}$ was found in [12], it is given by the formula

$$\Psi_{\kappa, -\infty, 1}(\mathbf{x}) = \kappa^{3/2}C_g e^{-|\kappa\mathbf{x}|^2/2}C e^{-|\mathbf{x}|}, \quad \omega_{\kappa, 1} = -\frac{1}{2} - \frac{1}{2}\kappa^2 \ln C^2, \quad (192)$$

where

$$C^{-2} = \frac{4}{\pi^{1/2}} \left[\frac{3}{4}\sqrt{\pi}e - \frac{3}{4}\sqrt{\pi} \operatorname{erf}(1)e - \frac{1}{2} \right], \quad \frac{1}{2}\ln C^2 \simeq 1.868.$$

Hence the nonlinear correction for the ground level is of order κ^2 .

Since the Palais-Smale condition is satisfied according to Theorem 5.4, the existence of an infinite sequence of discrete negative energy values of $\mathcal{E}_{\kappa, \xi}(\Psi)$ can be proven exactly along the lines of [9]. But we want to show, in addition, that the eigenvalues of the nonlinear problem with small κ are close to the eigenvalues of the linear problem (this is not surprising, since all the eigenvalues of the linear problem

for radial functions are simple). Therefore we modify the construction of critical points of the functional $\mathcal{E}_{\kappa,\xi}$ on Ξ .

We will use the following deformation lemma which is a minor modification and reformulation in our notation of Lemma 5 from [9] (with essentially the same proof).

Lemma 5.5. *Suppose that the functional $\mathcal{E}_{\kappa,\xi} \in C^1(\Xi_{\text{rad}}, \mathbb{R})$ satisfies Palais-Smale condition as in Theorem 5.4. Suppose also that $E'' < 0$ and that the segment $E' \leq E \leq E''$ does not contain critical values of $\mathcal{E}_{\kappa,\xi}$. Let $\bar{\epsilon} > 0$ be arbitrary small number. Then there exists $0 < \epsilon < \bar{\epsilon}$ and a mapping $\eta \in C(\Xi_{\text{rad}}, \Xi_{\text{rad}})$ such that*

- (i) $\eta(u) = u$ for $u \in \Xi_{\text{rad}}$ with $\mathcal{E}_{\kappa,\xi}(u) \leq E' - \bar{\epsilon}$ or $\mathcal{E}_{\kappa,\xi}(u) \geq E'' + \bar{\epsilon}$.
- (ii) η is a homeomorphism $\Xi_{\text{rad}} \rightarrow \Xi_{\text{rad}}$ and it is odd if $\mathcal{E}_{\kappa,\xi}$ is even.
- (iii) $\mathcal{E}_{\kappa,\xi}(\eta(u)) \leq \mathcal{E}_{\kappa,\xi}(u)$.
- (iv) $\eta(\{u \in \Xi_{\text{rad}} : \mathcal{E}_{\kappa,\xi}(u) \leq E + \epsilon\}) \subset \{u \in \Xi_{\text{rad}} : \mathcal{E}_{\kappa,\xi}(u) \leq E - \epsilon\}$ for $E \in [E', E'']$.

To prove existence of critical points of $\mathcal{E}_{\kappa,\xi}(\Psi)$ on the infinite-dimensional sphere Ξ_{rad} with critical values $E_n^{\kappa,\xi}$ near E_n^0 , $n = 2, 3, \dots$ when κ is small, we slightly modify the construction from [9]. As a first step we define finite-dimensional domain $B = B_n \subset L_n^-$ which lies in Ξ_{rad} near eigenfunction Ψ_n^0 of \mathcal{O}_{rad} as follows:

$$B_n = \left\{ \Psi : \Psi = (1 - R^2)^{1/2} \Psi_n^0 + v, v \in L_{n-1}^-, \|v\| = R, 0 \leq R \leq R_0 \right\}, \quad (193)$$

where $R_0 < 1/2$ is a small fixed number, for simplicity we fix $R_0 = 1/3$. The domain B_n is diffeomorphic to a $n - 1$ dimensional ball. The boundary of B_n is the $n - 2$ dimensional sphere

$$\partial B_n = \left\{ \Psi : \Psi = (1 - R_0^2)^{1/2} \Psi_n^0 + v, v \in L_{n-1}^-, \|v\| = R_0 \right\}. \quad (194)$$

We consider continuous functions Γ defined on B_n with values in Ξ . We consider the class $\{\Gamma\}_n$ of continuous mappings $\Gamma : B_n \rightarrow \Xi_{\text{rad}}$ such that Γ restricted to ∂B_n is identical,

$$\Gamma(\Psi) = \Psi \text{ if } \Psi \in \partial B_n. \quad (195)$$

The n -th min-max energy level $E_{\kappa,\xi,n}$ is defined as follows:

$$E_{\kappa,\xi,n} = \inf_{\Gamma \in \{\Gamma\}_n} \max_{\Psi \in B_n} \mathcal{E}_{\kappa,\xi}(\Gamma(\Psi)). \quad (196)$$

Lemma 5.6. *Let $\xi \leq 0$, let $n = 2, 3, \dots$, $0 < \kappa \leq 1$. Then $E_{\kappa,\xi,n}$ defined by (196) lies in the interval*

$$I_n = [E', E''], \text{ with } E' = E_n^0 - C_{3n} \kappa^2 (1 + |\ln \kappa|), \quad E'' = E_n^0 + C_{1n} \kappa^2, \quad (197)$$

where C_{1n} and C_{3n} depend only on n .

Proof. Since we can take a particular function $\Gamma(\Psi) = \Gamma_0(\Psi) = \Psi_n^0 + v$ for $\Psi \in B_n$ we have

$$E_{\kappa,\xi,n} \leq \max_{\Psi \in B_n} \mathcal{E}_{\kappa,\xi}(\Psi) \leq \mathcal{E}_0(\Psi_n^0) + \max_{B_n} \mathcal{G}_{\kappa,\xi}(\Psi) = E_n^0 + \max_{B_n} \mathcal{G}_{\kappa,\xi}(\Psi). \quad (198)$$

Note that B_n lies in a ball in a finite-dimensional subspace L_n^- in H^1 , the basis of L_n^- consists of exponentially decaying functions with bounded first derivatives, hence B_n is compact in $H^1(\mathbb{R}^3)$ and in $L^p(\mathbb{R}^3)$ for every $p \geq 1$. Therefore

$$\|\Psi\|_{H^1} + \|\Psi\|_{L^3} + \|\Psi\|_{L^{4/3}} \leq C_{0,n} \text{ for } \Psi \in B_n.$$

Hence, using (165) and power estimates for $\Psi^2 \ln \Psi^2$ we conclude that

$$\mathcal{G}_{\kappa,\xi}(\Psi) \leq \mathcal{G}_{\kappa,-\infty}(\Psi) \leq C \kappa^2 \left(\|\Psi\|_{L^3}^3 + \|\Psi\|_{L^{4/3}}^{4/3} \right) - \kappa^2 (\ln \kappa^{-3}/C_g^2 + 2) \|\Psi\|^2$$

and we obtain

$$\max_{B_n} \mathcal{G}_{\kappa, \xi}(\Psi) \leq C_{1n} \kappa^2, \quad (199)$$

where C_{1n} depends only on n . Using $\Gamma_0(\Psi)$ and the estimate (198) of $\mathcal{E}_{\kappa, \xi}(\Psi)$ we observe that

$$E_{\kappa, \xi, n} = \inf_{\Gamma \in \{\Gamma\}_n, \mathcal{E}_{\kappa, \xi}(\Gamma(B_n)) \leq C_{2n}} \max_{\Psi \in B_n} \mathcal{E}_{\kappa, \xi}(\Gamma(\Psi)), \quad (200)$$

where $C_{2n} = C_{1n} \kappa^2 + E_n^0$. Inequality (199) provides E'' in (197).

Now we estimate $E_{\kappa, \xi, n}$ from below. Mappings $\Gamma \in \{\Gamma\}_n$ which satisfy (195) have the following topological property: the set $\Gamma(B_n)$ must intersect the subspace L_{n-1}^+ . Indeed, assume that the contrary were true and for some Γ there were not intersection of $\Gamma(\Psi)$ with L_{n-1}^+ , that is $\|\Pi_{n-1}^+ \Gamma(\Psi)\| \neq 0$ for all $\Psi \in B_n$ where Π_{n-1}^- is the orthoprojection onto the finite-dimensional subspace L_{n-1}^- . Then we could consider the following function on the ball $\|v\| \leq R_0$ in L_{n-1}^- :

$$\Gamma_1(v) = \frac{R_0}{N(v)} \Pi_{n-1}^- \Gamma(v),$$

where $N(v) = \|\Pi_{n-1}^-(\Gamma(v))\|$. This function is continuous on the ball $\{\|v\| \leq R_0\}$ (since the denominator $N(v)$ does not vanish) and $\Gamma_1(v) = v$ if $\|v\| = R_0$, and also it has the property $\|\Gamma_1(v)\| = R_0$ if $\|v\| \leq R_0$. A function with such properties is called a retraction of the ball $\{\|v\| \leq R_0\}$ in the $(n-1)$ -dimensional space L_{n-1}^- onto its boundary $\{\|v\| = R_0\}$. It is a well-known fact from the algebraic topology that such a retraction cannot exist. Therefore for every Γ we have $\|\Pi_{n-1}^- \Gamma(\Psi_0)\| = 0$ for some $\Psi_0 \in B$. Therefore there exists $\Psi_0 \in B_n$ such that

$$\Gamma(\Psi_0) = (1 - R^2)^{1/2} \Psi_0^0 + w, \quad w \in L_n^+, \quad \|w\|^2 = R^2 \leq 1. \quad (201)$$

To obtain estimate of $E_{\kappa, \xi, n}$ from below note that (201) implies

$$\mathcal{E}_0(\Gamma(\Psi_0)) = (1 - R^2) \mathcal{E}_0(\Psi_0^0) + \mathcal{E}_0(w) \geq (1 - R^2) E_n^0 + E_n^0 \|w\|^2 \geq E_n^0.$$

Therefore, we obtain for $\Gamma \in \{\Gamma\}_n$, $\mathcal{E}_{\kappa, \xi}(\Gamma(B_n)) \leq C_{2n}$

$$\mathcal{E}_{\kappa, \xi}(\Gamma(\Psi_0)) \geq E_n^0 + \min_{\Psi \in \Xi, \mathcal{E}_{\kappa, \xi}(\Psi) \leq C_{2n}} \mathcal{G}_{\kappa, \xi}(\Psi).$$

Inequality $\mathcal{E}_{\kappa, \xi}(\Gamma(B_n)) \leq C_{2n}$ by Lemma 5.2 implies the boundedness $\Gamma(B_n)$ in H^1 . Using (iv) in Lemma 5.2 we conclude that

$$E_{\kappa, \xi, n} \geq E_n^0 - \kappa^2 C_{3n} (1 + |\ln \kappa|). \quad (202)$$

Combining (202), (198) and (199) we obtain (197). \square

Now we prove the existence of solutions of eigenvalue problem with regularized logarithm.

Theorem 5.7. *Let $-\infty < \xi \leq 0$. Let integer $n \geq 2$ and $\kappa \leq 1$ be so small that*

$$\frac{1}{9} (E_{n-1}^0 - E_n^0) + C_{1n} \kappa^2 + C_{3n} \kappa^2 (1 + |\ln \kappa|) < 0, \quad (203)$$

where E_n^0 are defined by (191) and C_{1n} is the constant from (199). Then

- (i) *the interval I_n defined by (197) contains a critical point $E_n^{\kappa, \xi}$ of $\mathcal{E}_{\kappa, \xi}$;*
- (ii) *there exists a solution $\Psi_n \in \Xi_{\text{rad}}$ of (172) with eigenvalue $\omega = \omega_{\kappa, \xi, n}$ such that $|E_n^{\kappa, \xi} - \omega_{\kappa, \xi, n}| \leq \frac{\kappa^2}{2}$ which satisfies*

$$|\omega_{\kappa, \xi, n} - \omega_{0, n}| \leq C_n \kappa^2 (1 + |\ln \kappa|). \quad (204)$$

Proof. We follow here the lines of [9] with minor modifications. Point (ii) follows from point (i) and (186). To prove (i) assume the contrary, namely let n and κ satisfy all the conditions and assume that the interval I_n defined by (197) does not contain critical points of $\mathcal{E}_{\kappa,\xi}$. We apply then Lemma 5.5 where we take

$$\bar{\epsilon} \leq \frac{1}{2} \left| \frac{1}{9} (E_{n-1}^0 - E_n^0) + C_{1n} \kappa^2 + C_{3n} \kappa^2 (1 + |\ln \kappa|) \right|,$$

with $E' = E_n^0 - \kappa^2 C_{3n} (1 + |\ln \kappa|)$ and find a mapping $\eta : \Xi_{\text{rad}} \rightarrow \Xi_{\text{rad}}$. By Lemma 5.6 the value $E_{\kappa,\xi,n}$ defined by (196) or (200) lies inside I_n . By point (iv) of Lemma 5.5

$$\eta(\{u \in \Xi_{\text{rad}} : \mathcal{E}_{\kappa,\xi}(u) \leq E_{\kappa,\xi,n} + \epsilon\}) \subset \{u \in \Xi_{\text{rad}} : \mathcal{E}_{\kappa,\xi}(u) \leq E_{\kappa,\xi,n} - \epsilon\}.$$

We can find $\Gamma \in \{\Gamma\}_n$ such that $\max_{B_n} \Gamma(\Psi) \leq E_{\kappa,\xi,n} + \epsilon/2$. If we consider $\Gamma'(\Psi) = \eta(\Gamma(\Psi))$ then we get $\max_{B_n} \Gamma'(\Psi) \leq E_{\kappa,\xi,n} - \epsilon/2$. To infer from this inequality a contradiction with definition (196) we have to check that $\Gamma' \in \{\Gamma\}_n$, namely to check (195). Note that on ∂B_n

$$\begin{aligned} & \mathcal{E}_0 \left((1 - R_0^2)^{1/2} \Psi_n^0 + v \right) \\ &= (1 - R_0^2) E_n^0 + \mathcal{E}_0(v) \leq E_n^0 + R_0^2 (E_{n-1}^0 - E_n^0), \end{aligned}$$

and hence

$$\begin{aligned} & \mathcal{E}_{\kappa,\xi} \left((1 - R_0^2)^{1/2} \Psi_2^0 + v \right) \\ & \leq E_n^0 + R_0^2 (E_{n-1}^0 - E_n^0) + \mathcal{G}_{\kappa,\xi} \left((1 - R_0^2)^{1/2} \Psi_n^0 + v \right). \end{aligned} \tag{205}$$

Therefore

$$\mathcal{E}_{\kappa,\xi}|_{\partial B_n} \leq E_n^0 + R_0^2 (E_{n-1}^0 - E_n^0) + \max_{\partial B_n} (\mathcal{G}_{\kappa,\xi}(\Psi)), \tag{206}$$

and using (199) and (203), since $R_0^2 = 1/9$, we conclude that

$$\mathcal{E}_{\kappa,\xi}|_{\partial B_n} \leq E_n^0 + R_0^2 (E_{n-1}^0 - E_n^0) + C_{1n} \kappa^2 \leq E' - \bar{\epsilon}. \tag{207}$$

implying $\eta(\Psi) = \Psi$ on ∂B_n by point (i) of Lemma 5.5. Hence, $\Gamma' \in \{\Gamma\}_n$ and we obtain a contradiction with (196). So we conclude that I_n contains a critical point Ψ' . Since $\mathcal{E}_{\kappa,\xi}$ is differentiable at Ψ' , this critical point provides a solution to (172), and (204) follows from (180). \square

Now we show that solutions of (172) decay exponentially as $r = |\mathbf{x}| \rightarrow \infty$.

Lemma 5.8. *Let $n \leq n_0$. Let $0 < \kappa \leq \kappa_0$ where κ_0 is small enough for conditions of Theorem 5.7 to be fulfilled for $n \leq n_0$. Let $\bar{\xi} \leq 0$ satisfy*

$$1 - \frac{\kappa^2}{4} |\bar{\xi}| + \frac{3\kappa^2}{2} < 0. \tag{208}$$

Let $p = \frac{\kappa}{3} |\bar{\xi}|^{1/2}$. Let $\Psi_n \in \Xi_{\text{rad}}$ be a solution of (172) with eigenvalue $\omega = \omega_{\kappa,\xi,n}$ which is described in Theorem 5.7 with $\xi \leq \bar{\xi}$. Then there exist positive constants R_1 and C which depend only on n_0 , κ and $\bar{\xi}$, such that for $\xi \leq \bar{\xi}$, $n \leq n_0$

$$|\Psi_n(r)| \leq C'' e^{-pr} \text{ for } r \geq R_1. \tag{209}$$

Proof. Since $\|\Psi_n\|_{H^1}$ are bounded uniformly in $\xi \leq 0$ and $\kappa \leq 1$ we can use the following result of Strauss (see Lemma A.II in [9])

$$|\Psi_n(r)| \leq C'_0 r^{-1} \|\Psi_n\|_{H^1} \text{ for } r \geq \bar{R}, \tag{210}$$

where C'_0 and \bar{R} are absolute constants, $\bar{R} \geq 1$. We apply this inequality to radial solutions $\Psi = \Psi_n$ of (172) with $\omega = \omega_{\kappa, \xi, n} < 0$ and obtain

$$|\Psi_n(r)| \leq C_0 r^{-1} \text{ for } r \geq \bar{R}, \quad (211)$$

where, according to Lemma 5.2, the constant C_0 is bounded uniformly in $\kappa \leq 1, \xi \leq 0$ and n . We write (172) in the form

$$\frac{1}{2} \nabla^2 \Psi + V_{\kappa, \xi} \Psi = 0, \quad (212)$$

where

$$V_{\kappa, \xi}(\mathbf{x}) = \frac{1}{|\mathbf{x}|} - \frac{1}{2} G'_{/\kappa, \xi}(|\Psi(\mathbf{x})|^2) + \omega.$$

According to (211) using monotonicity of the function $\ln_{+, \xi}(s)$ with respect to s we obtain for $|\mathbf{x}| \geq R \geq \bar{R} \geq 1$,

$$V_{\kappa, \xi}(\mathbf{x}) \leq \frac{1}{R} + \frac{\kappa^2}{2} (\ln_{+, \xi}(\kappa^{-3} R^{-2} C_0^2 / C_g^2) + 3) + \omega.$$

Note that

$$V_{\kappa, \xi}(\mathbf{x}) \leq \frac{1}{R} + \frac{\kappa^2}{2} (\xi + 3) + \omega \text{ if } \ln(\kappa^{-3} R^{-2} C_0^2 / C_g^2) \leq \xi, R \geq \bar{R}.$$

Therefore, for any $0 < \kappa \leq \kappa_0$, $\bar{\xi} \leq 0$ we can find $R_1 \geq \bar{R}$ such that

$$\ln(\kappa^{-3} R_1^{-2} C_0^2 / C_g^2) \leq \bar{\xi},$$

and if $|\bar{\xi}|$ is so large that (208) holds, we obtain for $\xi = \bar{\xi}$

$$V_{\kappa, \xi}(\mathbf{x}) \leq -\frac{\kappa^2}{4} |\bar{\xi}| + \omega < 0 \text{ for } |\mathbf{x}| \geq R_1. \quad (213)$$

According to definition (160) $V_{\kappa, \xi}(\mathbf{x})$ is a monotonely increasing function of ξ , therefore this inequality holds for all $\xi \leq \bar{\xi}$.

Note that $\Psi(\mathbf{x})$ cannot change sign for $|\mathbf{x}| > R_1$. Indeed, if $\Psi(\mathbf{x}) = 0$ at $|\mathbf{x}| = R'_1 > R_1$ we could multiply (212) by Ψ and integrate over $\{|\mathbf{x}| > R'_1\}$ which would yield

$$\int_{\{|\mathbf{x}| > R'_1\}} \left(\frac{1}{2} |\nabla \Psi|^2 - V_{\kappa, \xi}(\mathbf{x}) |\Psi|^2 \right) d\mathbf{x} = 0,$$

and $\Psi(\mathbf{x}) = 0$ for all $|\mathbf{x}| > R'_1$ which is impossible for a radial solution of (172) with $\|\Psi\| = 1$. So we assume $\Psi(\mathbf{x}) > 0$ for $|\mathbf{x}| > R_1$ (the case of negative Ψ is similar). We compare the solution Ψ of this equation in the domain $|\mathbf{x}| > R$ with the function

$$Y = C_Y \frac{1}{r} e^{-pr}, \quad p > 0, C_Y > 0,$$

which is a solution of the equation

$$\nabla^2 Y - p^2 Y = 0.$$

Subtracting half this equation from (212) we obtain

$$\frac{1}{2} \nabla^2 (\Psi - Y) + V_{\kappa, \xi}(\Psi - Y) + \left(V_{\kappa, \xi} + \frac{1}{2} p^2 \right) Y = 0. \quad (214)$$

We choose $p^2 = \frac{\kappa^2}{9} |\bar{\xi}|$ and (213) implies

$$\left(V_{\kappa, \xi} + \frac{1}{2} p^2 \right) < \omega < 0 \text{ for } |\mathbf{x}| \geq R_1. \quad (215)$$

We choose $C_Y > 0$ so that

$$C_Y e^{-pR_1} > C_0,$$

where C_0 is the same as in (211). We assert that

$$\Psi(\mathbf{x}) - Y(\mathbf{x}) \leq 0 \text{ for } |\mathbf{x}| \geq R_1. \quad (216)$$

This is true at $|\mathbf{x}| = R_1$ according to the choice of C_Y , the limit of $\Psi - Y$ as $|\mathbf{x}| \rightarrow \infty$ is zero. Assume now that (216) does not hold for some $|\mathbf{x}| > R_1$. Then $\Psi(\mathbf{x}) - Y(\mathbf{x})$ must have a point of local positive maximum at some $|\mathbf{x}| = R'_1 > R_1$, at this point $\nabla^2(\Psi - Y) \leq 0$, by (215) $(V_{\kappa,\xi} + p^2)Y < 0$ and $V_{\kappa,\xi}(\Psi - Y) \leq 0$ by (213). This inequalities contradict (214), hence (216) holds. Inequality (209) follows from (216). \square

Now we prove the main result of this section for the nonlinear eigenvalue problem with the original logarithmic inequality which corresponds to $\xi = -\infty$.

Theorem 5.9. *Let $\xi = -\infty$, $n_0 > 0$ and let integer $2 \leq n \leq n_0$ and $\kappa \leq 1$ be so small that (203) holds. Then there exists a solution $\Psi_n \in \Xi_{\text{rad}} \cap X$ of (172) with eigenvalue $\omega = \omega_{\kappa,n}$ with energy $E_n^\kappa = \omega_{\kappa,n} + \frac{\kappa^2}{2}$ which satisfies the inequality*

$$|\omega_{\kappa,n} - \omega_{0,n}| \leq C_n \kappa^2 (1 + |\ln \kappa|). \quad (217)$$

The solution Ψ_n decays superexponentially as $|\mathbf{x}| \rightarrow \infty$, namely (209), where R_1 depends on p , holds with arbitrary large p .

Proof. We fix n and consider a sequence $\xi_m \rightarrow -\infty$. We have a sequence of solutions $\Psi_{n,m} \in \Xi_{\text{rad}}$ of (172) with $\omega_{\kappa,\xi_m,n}$ satisfying (204) which exist according to Theorem 5.7 with $\xi = \xi_m$. Note that according to (197) $\mathcal{E}_\kappa(\Psi_{n,m}) \in [E', E'']$ are bounded uniformly in m . Therefore $\Psi_{n,m}$ are bounded in H^1 . Let us fix $\bar{\xi}$ which satisfies (208) and take such m that $\xi_m \leq \bar{\xi}$. All $\Psi_{n,m}$ satisfy (209). We can find a subsequence of $\Psi_{n,m}$ which converges to $\Psi_{n,\infty} \in \Xi_{\text{rad}}$ weakly in H^1 , strongly in $L^5(\{|\mathbf{x}| \leq R\}) \cap L^1(\{|\mathbf{x}| \leq R\})$ for every $R > 0$ and almost everywhere in \mathbb{R}^3 ; we also choose the subsequence so that $\omega_{\kappa,\xi_m,n} \rightarrow \omega_{\kappa,-\infty,n} \in [E', E''] - \frac{\kappa^2}{2}$. We obtain that $\nabla^2 \Psi_{n,m}$ converges weakly to $\nabla^2 \Psi_{n,\infty} \in \Xi_{\text{rad}}$. Now we show that $\Psi_{n,\infty}$ is a solution of (172) with $\omega = \omega_{\kappa,n} = \omega_{\kappa,-\infty,n}$ in the sense of distributions. The restriction of $g_{\kappa,\xi_m}(\Psi_{n,m}(\mathbf{x}))$ to the ball $\{|\mathbf{x}| \leq R\}$ converges to $g_{\kappa,-\infty}(\Psi_{n,\infty}(\mathbf{x}))$ in $L^2(\{|\mathbf{x}| \leq R\})$. Multiplying (172) with $\xi = \xi_m$ by an infinitely smooth test function f with compact support and integrating, we observe that we can pass to the limit in every term of the equation, obtaining that $\Psi_{n,\infty}$ is a solution of (172). Now we show that $\Psi_{n,\infty} \in \Xi_{\text{rad}} \cap X$. Since estimate (209) is uniform in $\xi_m \leq \bar{\xi}$ and $|G_{\kappa,-\infty}(C'' e^{-p r})|$ is integrable over \mathbb{R}^3 we easily derive from dominated convergence theorem that

$$\int_{|\mathbf{x}| \geq R_1} G_{\kappa,\xi_m}(\Psi_{n,m}) d\mathbf{x} \rightarrow \int_{|\mathbf{x}| \geq R_1} G_{\kappa,-\infty}(\Psi_{n,\infty}) d\mathbf{x}. \quad (218)$$

Note also that

$$\int_{|\mathbf{x}| \leq R_1} G_{\kappa,\xi_m}(\Psi_{n,m}) d\mathbf{x} \rightarrow \int_{|\mathbf{x}| \leq R_1} G_{\kappa,-\infty}(\Psi_{n,\infty}) d\mathbf{x} \quad (219)$$

as $m \rightarrow \infty$. Indeed,

$$\begin{aligned} & G_{\kappa,\xi_m}(|\Psi_{n,m}|^2) - G_{\kappa,-\infty}(|\Psi_{n,\infty}|^2) = \\ & = G_{\kappa,\xi_m}(|\Psi_{n,m}|^2) - G_{\kappa,-\infty}(|\Psi_{n,m}|^2) + G_{\kappa,-\infty}(|\Psi_{n,m}|^2) - G_{\kappa,-\infty}(|\Psi_{n,\infty}|^2) \end{aligned}$$

Note that $G_{\kappa, -\infty}(|\Psi|^2)$ defined by (49) satisfies Lipschitz condition.

$$\left| G_{\kappa, -\infty}(|\Psi_{n,m}|^2) - G_{\kappa, -\infty}(|\Psi_{n,\infty}|^2) \right| \leq C \|\Psi_{n,m} - \Psi_{n,\infty}\| \left(1 + |\Psi_{n,m}|^2 - |\Psi_{n,\infty}|^2 \right).$$

Hence

$$\begin{aligned} & \int_{|\mathbf{x}| \leq R} \left| G_{\kappa, -\infty}(|\Psi_{n,m}|^2) - G_{\kappa, -\infty}(|\Psi_{n,\infty}|^2) \right| d\mathbf{x} \quad (220) \\ & \leq C' \|\Psi_{n,m} - \Psi_{n,\infty}\| \left(1 + \|\Psi_{n,m}\|_{L^4}^2 + \|\Psi_{n,\infty}\|_{L^4}^2 \right) + C' \|\Psi_{n,m} - \Psi_{n,\infty}\|_{L^1(|\mathbf{x}| \leq R)} \end{aligned}$$

From (166) we obtain

$$\int_{|\mathbf{x}| \leq R} \left| G_{\kappa, \xi_m}(|\Psi_{n,m}|^2) - G_{\kappa, -\infty}(|\Psi_{n,m}|^2) \right| d\mathbf{x} \leq C e^{\xi_m/4} \int_{|\mathbf{x}| \leq R} |\Psi_{n,m}| d\mathbf{x}. \quad (221)$$

Using (220), (221) and convergence of $\Psi_{n,m}$ in $L^1(\{|\mathbf{x}| \leq R\})$ we obtain (219). From (218) and (219) we infer

$$\int_{\mathbb{R}^3} G_{\kappa, \xi_m}(\Psi_{n,m}) d\mathbf{x} \rightarrow \int_{\mathbb{R}^3} G_{\kappa, -\infty}(\Psi_{n,\infty}) d\mathbf{x}. \quad (222)$$

This implies that $\Psi_{n,\infty} \in X$ with X defined by (137). From (222) and weak convergence in H^1 we infer that

$$\mathcal{E}_\kappa(\Psi_{n,\infty}) \leq \lim_{m \rightarrow \infty} \sup \mathcal{E}_\kappa(\Psi_{n,m}).$$

Since $\mathcal{E}_\kappa(\Psi_{n,m})$ are bounded uniformly, $\mathcal{E}_\kappa(\Psi_{n,\infty})$ is bounded, hence $\Psi_{n,\infty} \in W$. Therefore (172) holds in $H^{-1} + X'$. Similarly to (222) we obtain that $\|\Psi_{n,m}\|^2 \rightarrow \|\Psi_{n,\infty}\|^2 = 1$, hence $\Psi_{n,\infty} \in \Xi_{\text{rad}}$. Since we can choose $\bar{\xi}$ arbitrary large, p in (209) can also be taken arbitrary large, and from convergence almost everywhere we derive that $\Psi_{n,\infty}(r)$ decays superexponentially. \square

The following theorem shows, roughly speaking, that there is no eigenvalues ω of the nonlinear problem in the gaps between small neighborhoods of eigenvalues of the linear problem..

Theorem 5.10. *Let ω satisfy the inequalities*

$$-\frac{1}{2} \leq \omega_{0,n} + \delta < \omega < \omega_{0,n+1} - \delta < 0, \quad (223)$$

where $\delta > 0$. There exists $C_4(n) > 0$ such that if

$$\delta \geq C_4(n) \kappa^2 (1 + |\ln \kappa|), \quad (224)$$

then the set of (radial or non-radial) solutions $\Psi \in \Xi \cap X$ of equation (172) with such ω is empty.

Proof. Consider in $L^2(\mathbb{R}^3)$ a linear operator \mathcal{O}_ω (the classical Schrödinger operator with the Coulomb potential shifted by ω)

$$\mathcal{O}_\omega \Psi = \mathcal{O}\Psi - \omega\Psi = -\omega\Psi - \frac{1}{2}\nabla^2\Psi - \frac{1}{|\mathbf{x}|}\Psi.$$

Consider solution of (172) written in the form

$$\mathcal{O}_\omega \Psi = -\frac{1}{2}g_\kappa(\Psi) \quad (225)$$

with ω in the gap between two consecutive points of spectrum of \mathcal{O} . Multiplying (172) (where $\xi = -\infty$) in $H = L^2(\mathbb{R}^3)$ by $\Psi \in \Xi \cap X$ we obtain

$$\langle \mathcal{O}_\omega \Psi, \Psi \rangle = -\frac{1}{2} \langle g_\kappa(\Psi), \Psi \rangle, \quad (226)$$

where $g_\kappa(\Psi)$ is defined in (181), $\langle u, v \rangle$ coincides with scalar product in $H = L^2(\mathbb{R}^3)$ and determines duality between H^1 and H^{-1} and X and X' in (137). Note that $g_\kappa(\Psi) \in X'$ according to Lemma 9.3.3 in [15], hence the expressions are well-defined. Since

$$\int \frac{1}{|\mathbf{x}|} |\Psi|^2 d\mathbf{x} \leq C_\epsilon \|\Psi\|^2 + \epsilon \|\Psi\|_{H^1} \|\Psi\| \text{ for } \Psi \in H^1$$

with arbitrary small $\epsilon > 0$, we have

$$\langle \mathcal{O}_\omega \Psi, \Psi \rangle \geq \frac{1}{4} \|\Psi\|_{H^1}^2 - C'_\epsilon \|\Psi\|^2.$$

Using (128) we estimate $\langle g_\kappa(\Psi), \Psi \rangle$ and we obtain for solutions of (172) the following inequality:

$$\frac{1}{4} \|\Psi\|_{H^1}^2 - C'' \|\Psi\|^2 \leq \frac{3}{2} \kappa^2 \left| \ln \int |\nabla \Psi|^2 d\mathbf{x} \right|.$$

Hence $\|\Psi\|_{H^1} \leq M$ for solutions $\Psi \in \Xi \cap X$.

Let $\check{E}_n^0 \subset H^1(\mathbb{R}^3)$ be the finite-dimensional space with the orthonormal basis of eigenfunctions $\check{\Psi}_j$ of the operator $\mathcal{O}_0 = \mathcal{O}$ with negative eigenvalues $\check{\omega}_j \leq \omega_{0,n}$ (since we are not restricted to radial functions, the eigenvalues $\check{\omega}_j \leq \check{\omega}_{j+1}$ may have high multiplicity and $\check{\omega}_n < \omega_{0,n}$ for $n > 2$). Let Π_n be orthoprojection in $L^2(\mathbb{R}^3)$ onto \check{E}_n^0 . We have by (223)

$$\langle (\mathcal{O}_\omega - \mathcal{O}_\omega \Pi_n) \Psi, \Psi \rangle \geq (\omega_{0,n+1} - \omega) \|\Psi\|^2.$$

Since the eigenfunctions $\check{\Psi}_j$ of \mathcal{O} are bounded, continuous and decay exponentially, we see that operators

$$\Pi_n \Psi = \sum_{j=1}^n \langle \Psi, \check{\Psi}_j \rangle \check{\Psi}_j, \quad \mathcal{O}_\omega \Pi_n \Psi = \sum_{j=1}^n (\check{\omega}_j - \omega) \langle \Psi, \check{\Psi}_j \rangle \check{\Psi}_j$$

are bounded from $L^p(\mathbb{R}^3)$ to $L^{p'}(\mathbb{R}^3)$ for any given $p, p', \infty \geq p \geq 1, \infty \geq p' \geq 1$. Solutions $\Psi \in \Xi \cap X'$ are bounded in H^1 , and by Sobolev imbedding in $L^6(\mathbb{R}^3)$.

Since $|g_\kappa(\Psi)| \leq C \kappa^2 (1 + |\ln \kappa|) (|\Psi|^{3/2} + |\Psi|^{1/2})$ we obtain

$$\|\Pi_n g_\kappa(\Psi)\| \leq C'' \kappa^2 (1 + |\ln \kappa|) \quad (227)$$

Multiplying (172) by $\Psi - \Pi_n \Psi$ we obtain

$$\langle \mathcal{O}_\omega \Psi, (\Psi - \Pi_n \Psi) \rangle = -\frac{1}{2} \langle g_\kappa(\Psi), (\Psi - \Pi_n \Psi) \rangle$$

Therefore

$$\begin{aligned} (\omega_{0,n+1} - \omega) \|(1 - \Pi_n) \Psi\|^2 &\leq -\frac{1}{2} \langle g_\kappa(\Psi), (\Psi - \Pi_n \Psi) \rangle \\ &\leq -\frac{1}{2} \int g_\kappa(\Psi) \Psi d\mathbf{x} + \frac{1}{2} \|\Pi_n g_\kappa(\Psi)\| \|\Psi\| \end{aligned} \quad (228)$$

Using (128) and (227) to estimate the right-hand side we obtain

$$(\omega_{0,n+1} - \omega) \|(1 - \Pi_n) \Psi\|^2 \leq C_1 \kappa^2 (1 + |\ln \kappa|). \quad (229)$$

Multiplying (225) by $\Pi_n \Psi$ we obtain

$$\begin{aligned} |\omega_{0,n} - \omega| \|\Pi_n \Psi\|^2 &\leq |\langle \mathcal{O}_\omega \Psi, \Pi_n \Psi \rangle| = \frac{1}{2} |\langle \Pi_n g_\kappa(\Psi), \Pi_n \Psi \rangle| \\ &\leq \frac{1}{2} \|\Pi_n g_\kappa(\Psi)\| \leq C_2 \kappa^2 (1 + |\ln \kappa|). \end{aligned} \quad (230)$$

From (229) and (230) using (223) we obtain

$$\delta \|\Psi\|^2 \leq C_3 \kappa^2 (1 + |\ln \kappa|)$$

If we take in (224) $C_4(n) = 2C_3$ we obtain a contradiction with $\|\Psi\| = 1$. Hence, a solution of (172) with such ω does not exist. \square

Remark 6. Theorem 5.9 states that for every energy level of the linear Schrödinger hydrogen operator there exists an energy level of nonlinear hydrogen equation with the Coulomb potential with an estimate of difference of order $\sim \kappa^2 \ln \kappa$. Based on (173) we see that if $\chi = \hbar$ where \hbar is the Planck constant and $\kappa = 0$ then $\omega^1 = \omega_n^1$ coincide with standard expression for hydrogen frequencies, and a natural choice for parameter χ is $\chi = \hbar$.

Remark 7. A theorem similar to Theorem 5.9 (without superexponential decay of solutions) can be proven not only for the logarithmic nonlinearity, but for more general subcritical nonlinearities which involve a small parameter κ . Moreover, if corresponding functions g_κ are of class C^1 and their derivatives satisfy natural growth conditions, then the standard bifurcation analysis shows that every E_n^0 generates a branch $E_{\kappa,n}$ of solutions $\Psi_n \in \Xi_{\text{rad}}$ of (172) for small κ .

Remark 8. In Theorem 2.1 we assumed in the macroscopic case electron size a to be very small and in this section we assume $\kappa = a_1/a$ to be very small, which seem to contradict one another. But a closer look shows that in fact the both cases are consistent one with another, if we assume the possibility $a_1 \rightarrow 0$. To show that this assumption is quite reasonable, we look at the values of physical constants. Note that a typical macroscopic scale is $a_{\text{macr}} \sim 10^{-3} m$ and the Bohr radius $a_1 \sim 5.3 \times 10^{-11} m$. Note also that the error in (82) is of order $a^2/a_{\text{macr}}^2 \ll 1$ and here $\kappa^2 = a_1^2/a^2 \ll 1$ which is possible if $a_1^2 \ll a^2 \ll a_{\text{macr}}^2$. Since $a_1^2/a_{\text{macr}}^2 \sim 2.8 \times 10^{-15}$ we consider $a_1^2/a_{\text{macr}}^2 \rightarrow 0$ as a reasonable approximation.

Remark 9. In the case when the energy functional with the Coulomb potential $\mathcal{E}_{\text{Cb}}(\Psi)$ is considered not only on radial functions, the eigenvalues of the linear problem are not simple and have very high degeneracy. Note that if we start from the relativistic equation (13) and look for ω -harmonic solutions we arrive to a nonlinear perturbation of so-called *relativistic Schrödinger equation*, see [34]. The spectrum of this linear problem has a fine structure and the degeneracy with respect to the total angular momentum disappears. If we fix the value of z -component L_z of the angular momentum L , for example by looking for solutions of the form $\Psi_1 = e^{im_z \theta} \Psi_{10}(r, z)$ with a fixed integer m_z , one can eliminate the remaining degeneracy in the linear problem. This provides a ground to expect that the lower energy levels of the nonlinear relativistic Schrödinger equation can be approximated by the lower energy levels of the linear relativistic Schrödinger equation if κ is small.

Remark 10. Note that the decoupled equation (152) with $b = 0$ for proton has a unique ground state solution (gausson) which corresponds to the minimum E_1^p of energy (see Theorem 3.4) and has a sequence of solutions with higher critical energy levels E_j^p , $j \geq 2$ (see [14]). Since the ground state is unique, $E_j^p > E_1^p$ if $j > 1$.

The logarithmic nonlinearity $G'_2(|\psi|^2) = -\kappa_p^2 \ln(\kappa_p^{-3} |\psi|^2 / C_g^2) - 3$ for proton involves the parameter κ_p which is different from the parameter κ for electron. A simple rescaling and use of (122) shows that dependence of $E_n^p(\kappa_p)$ on κ_p is very simple: $E_n^p(\kappa_p) = \kappa_p^2 E_n^p(1)$. There are physical motivations based on experimental estimates of the size of the proton to assume that κ_p is large, $\kappa_p \gg 1$. So we can assume that the gap $E_j^p(\kappa_p) - E_1^p(\kappa_p) \geq (E_j^p(1) - E_1^p(1)) \kappa_p^2$ is larger than 1 for $j \geq 2$. (Numerically calculated values of $E_2^p(1) - E_1^p(1)$ are given in [13], they are of order 1). At the same time $\omega_{0,n}$ given by (191) satisfy inequality $-\frac{1}{2} \leq \omega_{0,n} < 0$. Consequently, since the total energy \mathcal{E} defined by (144) of the system (141)-(143) equals the sum of energies of electron and proton one may expect for small b and κ and large κ_p that the lower negative energy levels of the functional \mathcal{E} cannot branch as b varies from $E_j^p + \omega_{0,n}$ with $j \geq 2$ and must branch from $E_1^p + \omega_{0,n}$. Hence we expect that if b and κ are small and κ_p is large, the lower negative energy levels of the functional \mathcal{E} which corresponds to the system (141)-(143) are close to lower discrete energy levels of \mathcal{E}_{Cb} which are described in Theorem 5.9.

Acknowledgment. The research was supported through Dr. A. Nachman of the U.S. Air Force Office of Scientific Research (AFOSR), under grant number FA9550-04-1-0359.

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